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FILE COVERS 1907 - 14 Oct 2008 VOL 149 ISS 16 FILE LAST UPDATED: 12 Oct 2008 (20081012/ED)

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Structure attributes must be viewed using STN Express query preparation.

L3 195 SEA FILE=REGISTRY SSS FUL L1 L4 50 SEA FILE=CAPLUS L3

=> d 14 1-50 ibib abs hitstr

L4 ANSWER 1 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:829945 CAPLUS

DOCUMENT NUMBER: 149:153074

TITLE: Preparation of pyridines and pyrimidines as JNK and

ERK kinase inhibitors

INVENTOR(S): Belanger, David B.; Siddiqui, M. Arshad; Curran, Patrick J.; Hamann, Blake; Zhao, Lianyun; Reddy,

Panduranga Adulla P.; Tadikonda, Praveen K.; Shipps,

Gerald W., Jr.; Mansoor, Umar Faruk

PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: PCT Int. Appl., 243pp.

CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE:

Patent English : 1

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAT	PATENT NO.						DATE			APPL	ICAT	ION	NO.		D	ATE	
						-											
WO	2008	0824	87		A2		2008	0710		WO 2	007-	JS25	764		2	0071	217
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		CH,	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DO,	DZ,	EC,	EE,	EG,	ES,	FI,
		GB,	GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,
		KM,	KN,	KP,	KR,	ΚZ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LY,	MA,	MD,	ME,
		MG,	MK,	MN,	MW,	MX,	MY,	ΜZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,
	MG, MK, MI PT, RO, R					SC,	SD,	SE,	SG,	SK,	SL,	SM,	SV,	SY,	TJ,	TM,	TN,
		TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	ZA,	ZM,	ZW				
	RW:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,
		IS,	IT,	LT,	LU,	LV,	MC,	MT,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,
		ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,
		GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,
	BY, KG, K						TJ,	TM									
PRIORITY	PRIORITY APPLN. INFO.:									US 2	006-	8761	04P	1	P 2	0061	220
OTHER SO	THER SOURCE(S):						149:	1530	74								

GI

AB Title compds. [I, X = N, CH; Y = N, CR5; Rla = H, halo, OH, alkoxy, alkyl, (substituted) aryl, heteroaryl, amino; R2a = H, halo, alkyl, OH, alkoxy, amino; R3 = H, halo, alkyl, cycloalkyl, (substituted) aminocarbonyl, aryl, heteroaryl, amino, etc.; R4 = (substituted) aminocarbonyl, aryl, heteroaryl, heterocycloalkyl, amino, etc.; R5 = H, halo, OH, alkoxy, amino], were prepared Thus, title compound (II) (preparation outlined) inhibited

- JNK1 with IC50 = 4 nM.
- IT 1038409-10-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyridines and pyrimidines as JNK and ERK kinase inhibitors) RN = 1038409-10-7 CAPLUS

CN 2-Pyridinecarboxamide, 6-[4-(4-fluorophenyl)-1H-pyrazol-1-yl]-N-[[4-(methylsulfonyl)phenyl]methyl]- (CA INDEX NAME)

1038408-88-6P 1038408-89-7P RL: PRPH (Prophetic); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyridines and pyrimidines as JNK and ERK kinase inhibitors) RN 1038408-88-6 CAPLUS

CN

2-Pyridinecarboxamide, 6-[4-(3-fluorophenyl)-1H-pyrazol-1-yl]-N-[[1-[4-(methylsulfonyl)phenyl]-1H-pyrazol-4-yl]methyl]- (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 1038408-89-7 CAPLUS

CN 2-Pyridinecarboxamide, 6-[4-(4-fluorophenyl)-1H-pyrazol-1-yl]-N-[[1-[4-(methylsulfonyl)phenyl]-1H-pyrazol-4-yl]methyl]- (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

L4 ANSWER 2 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:829152 CAPLUS

DOCUMENT NUMBER: 149:153073

TITLE: Heterocyclic carboxamide derivatives as calpain inhibitors and their preparation, pharmaceutical compositions and use in the treatment of diseases Kling, Andreas; Hornberger, Wilfried; Mack, Helmut;

INVENTOR(S): Moeller, Achim; Nimmrich, Volker; Seemann, Dietmar;

Lubisch, Wilfried PATENT ASSIGNEE(S): Abbott G.m.b.H. & Co. K.-G., Germany

SOURCE: PCT Int. Appl., 145pp.

CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

P.	ATENT	NO.			KIN	D	DATE			APPL	ICAT	ION :	.OV		D.	ATE	
-						-									-		
W	0 2008	0809	69		A1		2008	0710		WO 2	007-	EP64	617		2	0071	228
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		CA,	CH,	CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DO,	DZ,	EC,	EE,	EG,	ES,
		FI,	GB,	GD,	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,
		KG,	KM,	KN,	KΡ,	KR,	KZ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LY,	MA,	MD,
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	RW:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	ΙE,
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		BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM									
U	S 2008	0234	329		A1		2008	0925		US 2	008-	7094	1		2	0080	222
U	S 2008	0234	330		A1		2008	0925		US 2	-800	7206	5		2	0080	222
PRIORI	TY APP	LN.	INFO	. :						EP 2	006-	1273	69		A 2	0061	229
										WO 2	007-	EP64	617		A1 2	0071	228

OTHER SOURCE(S): MARPAT 149:153073

GT

The invention relates to carboxamide derivs. of formula I and their use for the manufacture of a medicament. The carboxamide compds. are inhibitors of calpain (calcium dependent cysteine proteases). The invention therefore also relates to the use of these carboxamide compds. for treating a disorder associated with an elevated calpain activity. Compds. of formula I wherein , R1 is H, (un)substituted C1-10 alkyl, (un)substituted C2-10 alkenyl, (un)substituted C2-10 alkynyl, C3-7 (hetero)cycloalkyl, C3-7 (hetero)cycloalkyl-C1-4 alkyl, etc.; R2 is H, (un)substituted C1-10 alkyl, (un) substituted C1-10 alkoxy, (un) substituted C2-10 alkenyl, (un) substituted C2-10 alkynyl, (un) substituted C3-7 (hetero) cycloalkyl, etc.; R3a and R3b are independently OH and C1-4 alkoxy; R3aR3b may taken together with the carbon attached to form C=O; X is H, CO2H and derivs., CONH2 and derivs., CONH-C1-6 alkyl and derivs. and CONH-NH2 and derivs.; Y is a divalent, (un) substituted aromatic or (un) substituted 6-membered heteroarom, radical; Y is a divalent, (un) substituted aromatic or (un) substituted 6-membered heteroarom, radical; W is (un) substituted imidazolyl and (un)substituted pyrazolyl; W and R2 may take together to form (un) substituted heterobi- or heterotricyclic radical; and their tautomers, prodrugs and pharmaceutically suitable salts thereof, are claimed. Example compound II was prepared via amidation of 2-(4-phenyl-1H-imidazol-1-yl)pyridine-3-carboxylic acid with 3-amino-2-hydroxyheptanamide; the resulting N-[1-(2-amino-1-hydroxy-2-oxoethyl)pentyl]-2-(4-phenyl-1H-imidazol-1yl)pyridine-3-carboxamide underwent oxidation to give II. All the invention compds. were evaluated for their calpain inhibitory activity. From the assay, it was determined that II exhibited the Ki values of ≤ 40 nM. 1037826-41-7P, N-[1-[Amino(oxo)acetyl]pentyl]-2-(4-phenyl-1Hpvrazol-1-vl)nicotinamide 1037826-42-8P, N-(3-Amino-1-benzyl-2,3-dioxopropyl)-2-(4-phenyl-1H-pyrazol-1vl)nicotinamide 1037827-46-5P, N-[3-Amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-[4-(2-fluorophenyl)-1Hpyrazol-1-yl]pyridine-3-carboxamide RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of heterocyclic carboxamide derivs. as calpain inhibitors useful in the treatment of diseases)

- RN 1037826-41-7 CAPLUS
- CN INDEX NAME NOT YET ASSIGNED

- RN 1037826-42-8 CAPLUS
- CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-(4phenyl-1H-pyrazol-1-yl)- (CA INDEX NAME)

- RN 1037827-46-5 CAPLUS
- CN 3-Pyridinecarboxamide, N-[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]-2-[4-(2-fluorophenyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)

$$\begin{array}{c|c} & \text{CH}_2\text{-Ph} \\ & \text{C-NH-CH-C-C-NH}_2 \\ \\ & \text{N} \\ & \text{N} \end{array}$$

- 1037828-51-5P, N-[1-(2-Amino-1-hydroxy-2-oxoethyl)pentyl]-2-(4phenyl-1H-pyrazol-1-yl)pyridine-3-carboxamide 1037828-52-6P, N-[3-Amino-2-hydroxy-3-oxo-1-(phenylmethyl)propyl]-2-(4-phenyl-1H-pyrazol-1-y1)pyridine-3-carboxamide RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 - (Reactant or reagent)
 - (intermediate; preparation of heterocyclic carboxamide derivs. as calpain inhibitors useful in the treatment of diseases) 1037828-51-5 CAPLUS
- RN

CN 3-Pyridinecarboxamide, N-[1-(2-amino-1-hydroxy-2-oxoethy1)penty1]-2-(4-phenyl-1H-pyrazol-1-y1)- (CA INDEX NAME)

- RN 1037828-52-6 CAPLUS
- CN 3-Pyridinecarboxamide, N-[3-amino-2-hydroxy-3-oxo-1-(phenylmethyl)propyl]-2-(4-phenyl-1H-pyrazol-1-yl)- (CA INDEX NAME)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:500481 CAPLUS

DOCUMENT NUMBER: 148:472035

TITLE: Preparation of acylaminopyrazoles as thrombin

inhibitors

INVENTOR(S):

Bauser, Marcus; Buchmueller, Anja; Degenfeld, Georges;
Dittrich-Wengenroth, Elke; Gerdes, Christoph, Gnoth,
Mark Jean; Gottschling, Dirk; Heitmeier, Stefan;
Hendrix, Martin; Koebberling, Johannes; Lang, Dieter;

Rester, Ulrich; Saatmann, Uwe; Tersteegen, Adrian; Bruens, Astrid

PATENT ASSIGNEE(S): Bayer HealthCare A.-G., Germany

SOURCE: PCT Int. Appl., 96pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent

DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	ENT :	NO.			KIN	D	DATE			APPL	ICAT	ION :	NO.		D	ATE	
						-									-		
WO	2008	0465	27		A1		2008	0424		WO 2	007-	EP86	57		2	0071	005
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		CH,	CN.	CO.	CR.	CU.	CZ.	DE.	DK.	DM.	DO.	DZ.	EC,	EE,	EG.	ES.	FI.

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GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG,
             KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME,
            MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL,
             PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN,
             TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG, BW,
             GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM
     DE 102006048924
                          Α1
                                20080424
                                            DE 2006-102006048924
                                                                    20061017
PRIORITY APPLN. INFO.:
                                            DE 2006-102006048924A 20061017
OTHER SOURCE(S):
                         MARPAT 148:472035
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R6 N N N N Pr-i O N N N Ph II

Pr-i O N

III

IT 1020653-18-2P 1020653-20-6P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of acylaminopyrazoles as thrombin inhibitors)

RN 1020653-18-2 CAPLUS

CN Benzeneacetamide, α,3,4-trimethoxy-N-(1-methylethyl)-N-[2-oxo-2-[[4-phenyl-1-(2-pyridinyl)-1H-pyrazol-3-yl]amino]ethyl]- (CA INDEX NAME)

RN 1020653-20-6 CAPLUS

CN Benzeneacetamide, 4-fluoro- α -methoxy-N-(1-methylethyl)-N-[2-oxo-2-[[4-phenyl-1-(2-pyridinyl)-1H-pyrazol-3-yl]amino]ethyl]- (CA INDEX NAME)

IT 1020653-52-4P 1020653-57-9P 1020653-62-6P
 RI: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of acylaminopyrazoles as thrombin inhibitors)

RN 1020653-52-4 CAPLUS

CN 1H-Pyrazol-3-amine, 4-phenyl-1-(2-pyridinyl)- (CA INDEX NAME)

RN 1020653-57-9 CAPLUS

CN Acetamide, 2-chloro-N-[4-phenyl-1-(2-pyridinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)

RN 1020653-62-6 CAPLUS

CN Acetamide, 2-[(1-methylethyl)amino]-N-[4-phenyl-1-(2-pyridinyl)-1H-pyrazol-3-yl]- (CA INDEX NAME)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:239735 CAPLUS

DOCUMENT NUMBER: 148:403118

TITLE: Base-Mediated Reaction of Hydrazones and Nitroolefins with a Reversed Regioselectivity: A Novel Synthesis of

1,3,4-Trisubstituted Pyrazoles
AUTHOR(S): Deng, Xiaohu; Mani, Neelakandha S.

CORPORATE SOURCE: Johnson & Johnson Pharmaceutical Research &

Development, L.L.C., San Diego, CA, 92121, USA

SOURCE: Organic Letters (2008), 10(6), 1307-1310 CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 148:403118

AB A regioselective synthesis of 1,3,4-tri- or 1,3,4,5-tetrasubstituted pyrazoles by the reaction of hydrazones with nitroclefins is described. Mediated with strong bases such as t-BuOK, the reaction exhibits a reversed, exclusive 1,3,4-regioselectivity. Subsequent quenching with strong acids such as TFA is essential to achieve good yields. A plausible

stepwise cycloaddn. reaction mechanism is proposed. 1016169-44-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(regioselective synthesis of 1,3,4-tri- or 1,3,4,5-tetrasubstituted pyrazoles by base-mediated reaction of hydrazones with nitroolefins

with reversed regioselectivity)

RN 1016169-44-0 CAPLUS

CN Pyridine, 2-[3-(4-chlorophenyl)-4-(4-methylphenyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)

L4 ANSWER 5 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:1300822 CAPLUS

DOCUMENT NUMBER: 147:533593

TITLE: A method for the preparation of maleimido derivatives

of biomolecule labeling reactants and conjugates

derived thereof INVENTOR(S): Hovinen, Jari

PATENT ASSIGNEE(S): Wallac Oy, Finland SOURCE: PCT Int. Appl., 31pp.

CODEN: PIXXD2 DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATE	ENT 1	.OV			KIN	D	DATE			APPL	ICAT	ION :	NO.		D.	ATE	
						-											
WO 2	2007:	1288	73		A1		2007	1115		WO 2	007-	FI50	247		2	0070	504
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		GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,
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IORITY	APPI	LN.	INFO	. :						FI 2	006-	5291			A 2	0060	505

PRIORITY APPLN. INFO.:

P 20060505

US 2006-797674P

US 2006-842036P

P 20060905

OTHER SOURCE(S):

CASREACT 147:533593; MARPAT 147:533593

ĠΙ

- AB This invention relates to a new method for the preparation of chelating agents or metal chelates, particularly lanthanide(III) chelates, tethered to a maleimido function and to novel end products and intermediates produced in said method. The chelating agents are maleimido derivs. (I) where L is a linking group and X is a chelating group. The invention concerns also biomol. conjugates derived thereof. Thus, the europium(III) chelate with a bis(aminomethyl)pyridine tetraacetate derivative (II) was prepared and was reacted with Ac-CVEIDK-COMPL to give the peptide conjugate.
 - T 189805-30-9 RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of lanthanide chelates of maleimido derivs. and their biomol. conjugates)

- RN 189805-30-9 CAPLUS
- CN Glycine, N,N'-[[4-[2-(4-aminophenyl)ethyl]-1H-pyrazole-1,3-diyl]bis(6,2-pyridinediylmethylene)]bis[N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-, 1,1'-bis(1,1-dimethylethyl) ester (CA INDEX NAME)

- IT 935687-82-4P
 - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of lanthanide chelates of maleimido derivs. and their biomol. conjugates)

- RN 935687-82-4 CAPLUS
- CN Glycine, N,N'-[[4-[2-[4-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-y1)-1-oxohexyl]amino]phenyl]ethyl]-1H-pyrazole-1,3-diyl]bis(6,2-pyridinediylmethylene)]bis[N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-,1,1'-bis(1,1-dimethylethyl) ester (CA INDEX NAME)

PAGE 2-A

REFERENCE COUNT: THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:770584 CAPLUS DOCUMENT NUMBER:

148:495841

TITLE: Synthesis and general bioactivity of 4-(3,4,5-trimethoxyphenyl)pyrazoles

Fielder, Layne M.; Smith, Stanton Q. AUTHOR(S):

Department of Chemistry, Virginia Military Institute, CORPORATE SOURCE: Lexington, VA, 24450, USA Journal of Undergraduate Chemistry Research (2007),

SOURCE:

6(2), 77-80 CODEN: JUCRBV; ISSN: 1541-6003

PUBLISHER: Virginia Military Institute

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 148:495841

Seven new 4-(3,4,5-trimethoxyphenyl)pyrazoles have been prepared by the reaction of various monosubstituted hydrazines with a vinamidinium salt. The pyrazoles were prepared in good to excellent yield and purity under mild conditions. Several of these pyrazoles exhibited activity in the brine shrimp assay.

IT 1021424-60-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis and general bioactivity of

4-(3,4,5-trimethoxyphenyl)pyrazoles)

RN 1021424-60-1 CAPLUS

CN Pyridine, 2-[4-(3,4,5-trimethoxyphenyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)

REFERENCE COUNT:

11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:619866 CAPLUS

DOCUMENT NUMBER: 147:52699
TITLE: Phenoxyac

TITLE: Phenoxyacetic acid derivatives as CRTH2 receptor ligands, their preparation, pharmaceutical

compositions, and use in therapy Ulven, Trond; Frimurer, Thomas; Rist, Oeystein;

INVENTOR(S): Ulven, Trond; Frimurer, Thomas; Rist, Oeystein; Kostenis, Evi; Hoegberg, Thomas; Receveur, Jean-Marie;

Grimstrup, Marie

PATENT ASSIGNEE(S): 7TM Pharma A/S, Den. SOURCE: PCT Int. Appl., 22pp.

English

SOURCE: PCT Int. Appl
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE:

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA:	TENT :	NO.			KIN	D	DATE		- 1	APPL	ICAT	ION	NO.		D	ATE	
						-											
WO	2007	0626	78		A1		2007	0607	1	WO 2	005-1	EP12	881		2	0051	129
	W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KN,	KP,	KR,
	KZ, LC			LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,	MN,	MW,	MX,
	KZ, LC, MZ, NA,			NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,
		SG,	SK,	SL,	SM,	SY,	TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,
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		IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	BJ,
		CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,
GM, KE,			KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
		KG,	KZ,	MD,	RU,	TJ,	TM										

PRIORITY APPLN. INFO.:

WO 2005-EP12881 20051129

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The invention relates to phenoxyacetic acid derivs. as CRTH2 (chemoattractant receptor-homologous mol. expressed on T helper cells type 2) receptor modulators. The invention also relates to the preparation of the compds. of the invention, pharmaceutical compns. comprising a compound of the invention together with a pharmaceutically acceptable carrier, as well as to the use of the compns. for the treatment of diseases responsive to modulation of CRTH2 receptors, particularly diseases having a significant inflammatory component, such as asthma. Ring opening and heterocyclization of chromone I with (3,5-dichloropyridin-2-y1)hydrazine gave phenol II, which underwent substitution of Et bromoacetate and hydrolysis to form phenoxyacetic acid III. The compds. of the invention, e.g., III, express IC50 values below 0.5 µM in assays for CRTH2 binding and CRTH2 antagonist function.

939437-70-4P, 4-Bromo-2-[[1-(3,5-dichloropyridin-2-yl)-1H-pyrazol-4-yl]carbonyl]phenoxyacetic acid

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of phenoxyacetic acid derivs. as CRTH2 receptor ligands)

RN 939437-70-4 CAPLUS

CN Acetic acid, 2-[4-bromo-2-[[1-(3,5-dichloro-2-pyridinyl)-1H-pyrazol-4vl]carbonyl]phenoxy]- (CA INDEX NAME)

939437-68-0P, (5-Bromo-2-hydroxyphenyl)[1-(3,5-dichloropyridin-2yl)-1H-pyrazol-4-yl]methanone 939437-69-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of phenoxyacetic acid derivs. as CRTH2 receptor ligands)

939437-68-0 CAPLUS RN

CM Methanone, (5-bromo-2-hydroxyphenyl)[1-(3,5-dichloro-2-pyridinyl)-1H- pyrazo1-4-y1]- (CA INDEX NAME)

939437-69-1 CAPLUS Acetic acid, 2-[4-bromo-2-[[1-(3,5-dichloro-2-pyridinyl)-1H-pyrazol-4-CN yl]carbonyl]phenoxy]-, ethyl ester (CA INDEX NAME)

REFERENCE COUNT:

TITLE:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2007:485399 CAPLUS

3

DOCUMENT NUMBER: 146:482057

Preparation of 5-aminopyrazoles as agricultural fungicides

INVENTOR(S): Huenger, Udo PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 73pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATI	ENT	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D.	ATE	
						-											
WO 2	2007	0487	33		A1		2007	0503		WO 2	006-	EP67	477		2	0061	017
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		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KN,
		KP,	KR,	KZ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,
		MN,	MW,	MX,	MY,	MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,
		RS,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	SV,	SY,	ТJ,	TM,	TN,	TR,	TT,
		TZ,	UA,	UG,	US,	UZ,	VC,	VN,	ZA,	ZM,	zw						
	RW:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,
		IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,
		CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,
		GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
		KG,	ΚZ,	MD,	RU,	ΤJ,	$^{\text{TM}}$										
PRIORITY	APP	LN.	INFO	. :						EP 2	005-	2358	6		A 2	0051	028
OTHER SOU	JRCE	(S):			MAR	PAT	146:	4820	57								
CT																	

GI

- AΒ Title compds. I [R1 = alkyl, haloalkyl, cycloalkyl, etc.; R2 = halo, CN, alkyl, etc.; X, Y, Z = N or CR3; R3 = H, halo, CN, etc.] were prepared For example, condensation of 2-chloro-6-hydrazinopyridine and 2-(1-oxopropvl)decanenitrile afforded aminopyrazole II in 96% vield.
- IT 935859-64-6P RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of 5-aminopyrazoles as agricultural fungicides)
- RN 935859-64-6 CAPLUS
- CN 1H-Pyrazol-5-amine, 1-(6-chloro-2-pyridiny1)-3-(3-methylbuty1)-4-(2phenylethyl) - (CA INDEX NAME)

L4 ANSWER 9 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:257547 CAPLUS

DOCUMENT NUMBER: 146:316909

TITLE: Preparation of anilinopyrazoles for the treatment of

diabetes

INVENTOR(S): Lowe, Derek; Shelekhin, Tatiana; Wang, Gan; Ma, Xin; Iwuagwu, Christiana; Ying, Shihong; Magnuson, Steven;

Rudolph, Joachim; Koebberling, Johannes;

Pernerstorfer, Josef; Mueller, Thomas; Brands,

Michael; Heimbach, Dirk; Lindner, Niels PATENT ASSIGNEE(S): Bayer Pharmaceuticals Corporation, USA

SOURCE: PCT Int. Appl., 165pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE . English

FAMILY ACC. NUM. COUNT:

ATEN	1T]	INFOR	MATI	: MC														
	PAT	TENT	NO.			KIN	D	DATE			APPL	ICAT	ION I	NO.		D	ATE	
							-											
	WO	2007	0278	42		A1		2007	0308		WO 2	006-	US33	957		2	0060	831
		W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,

MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,

GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM CA 2620425 A1 20070308 CA 2006-2620425 20060831 EP 1928455 A1 20080611 EP 2006-802675 20060831

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, RS

PRIORITY APPLN. INFO .: P 20050831 US 2005-713146P WO 2006-US33957 W 20060831

OTHER SOURCE(S): MARPAT 146:316909 GI

AR Title compds. [I; R = H, alkyl; R1 = H, (substituted) alkyl, cycloalkyl, haloalkyl, Ph, pyridyl; R2 = H, halo, (substituted) alkyl, cycloalkyl, haloalkyl, Ph, pyridyl, pyrimidyl, benzodioxolanyl; R3 = (Ph-fused) (substituted) 5-6 membered heteroaryl; R4 = alkyl, cycloalkyl, alkoxy,

haloalkyl, haloalkoxy, halo; n = 0-3; X = COZRB, CONRSR6, SOZNHRY; R5 = H, alkyl; (substituted) PhSO2; R6 = H, alkyl; R7 = H, Me; R8 = H, alkyl; with provisos], were prepared Thus, 2-[[1-(3,6-dimethylpyrazin-2-y1)-3-ethyl-apyridin-3-y1-1H-pyrazo1-5-y1]amino]5-methylbenzoic acid (preparation from 3-chloro-2,5-dimethylpyrazine, 3-oxopentamenitrile, Me

2-iodo-5-methylbenzoate, and 3-pyridineboronic acid given) and other I increased insulin secretion from dispersed rat islet cells by 0.8-6.8 fold

over controls.

1 928261-71-6P 928261-73-8P 928261-74-9P
928261-75-0P 928261-89-6P 928261-96-5P
928262-54-8P 928263-28-9P 928263-33-9P
928263-33-9P 928263-33-6P 928263-33-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (USes)

(preparation of anilinopyrazoles for the treatment of diabetes)

RN 928261-71-6 CAPLUS

CN Benzoic acid, 2-[[3-ethyl-1-(3-methyl-2-pyridinyl)-4-phenyl-1H-pyrazol-5-yl]amino]-5-methyl- (CA INDEX NAME)

RN 928261-73-8 CAPLUS

CN Benzoic acid, 2-[[3-ethyl-1-(3-methyl-2-pyridinyl)-4-phenyl-1H-pyrazol-5yl]amino]-5-(trifluoromethoxy)- (CA INDEX NAME)

RN 928261-74-9 CAPLUS

CN Benzoic acid, 2-[[3-ethyl-4-(3-fluorophenyl)-1-(3-methyl-2-pyridinyl)-1H-pyrazol-5-yl]amino]-5-(trifluoromethoxy)- (CA INDEX NAME)

RN 928261-75-0 CAPLUS
CN Benzoic acid, 2-[(4-(4-acetylphenyl)-3-ethyl-1-(3-methyl-2-pyridinyl)-1Hpyrazol-5-yl]aminoj-5-(trifluoromethoxy)- (CA INDEX NAME)

RN 928261-89-6 CAPLUS
CN Benzoic acid, 2-[[3-ethyl-4-(3-fluorophenyl)-1-(3-methyl-2-pyridinyl)-1Hpyrazol-5-yl]amino]-5-methyl- (CA INDEX NAME)

RN 928261-96-5 CAPLUS

 $\texttt{CN} \quad \texttt{Benzoic acid, 2-[[4-(2-fluorophenyl)-1-(3-methyl-2-pyridinyl)-3-propyl-1H-1]} \\$

pyrazol-5-yl]amino]- (CA INDEX NAME)

- RN 928262-54-8 CAPLUS
- CN Benzoic acid, 5-cyclopropyl-2-[[4-(2-fluorophenyl)-3-methyl-1-(3-methyl-2-pyridinyl)-1H-pyrazol-5-yl]amino]- (CA INDEX NAME)

- RN 928263-28-9 CAPLUS
- CN Benzoic acid, 2-[[3-ethyl-4-(2-methoxyphenyl)-1-(3-methyl-2-pyridinyl)-1H-pyrazol-5-yl]amino]-5-(trifluoromethoxy)- (CA INDEX NAME)

- RN 928263-30-3 CAPLUS
- ${\tt CN \quad Benzoic\ acid,\ 2-[[3-ethyl-4-[4-(methoxymethyl)phenyl]-1-(3-methyl-2-meth$

pyridiny1)-1H-pyrazo1-5-y1]amino]-5-(trifluoromethoxy)- (CA INDEX NAME)

RN 928263-32-5 CAPLUS

CN Benzoic acid, 2-[[4-(3-cyanopheny1)-3-ethyl-1-(3-methyl-2-pyridiny1)-1Hpyrazol-5-yl]amino]-5-(trifluoromethoxy)- (CA INDEX NAME)

RN 928263-33-6 CAPLUS

CN Benzoic acid, 2-[[4-(3-acetylphenyl)-3-ethyl-1-(3-methyl-2-pyridinyl)-1H-pyrazol-5-yl]amino]-5-(trifluoromethoxy)- (CA INDEX NAME)

RN 928263-34-7 CAPLUS

Benzoic acid, 2-[[3-ethyl-4-(4-methoxyphenyl)-1-(3-methyl-2-pyridinyl)-1H-CN pyrazol-5-yl]amino]-5-(trifluoromethoxy)- (CA INDEX NAME)

928264-33-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of anilinopyrazoles for the treatment of diabetes)

RN 928264-33-9 CAPLUS

CN Benzoic acid, 2-[[3-ethyl-4-(2-methoxyphenyl)-1-(3-methyl-2-pyridinyl)-1Hpyrazol-5-yl]amino]-5-(trifluoromethoxy)-, methyl ester (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 10 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER:

2007:247504 CAPLUS

DOCUMENT NUMBER: 146:478087

TITLE: Convenient Synthesis of Maleimido-Derivatized

Lanthanide(III) Chelates and Their Use in Mercapto

Group Conjugation AUTHOR(S): Hovinen, Jari

CORPORATE SOURCE: PerkinElmer Life and Analytical Sciences, Turku, FIN-20101, Finland

SOURCE: Bioconjugate Chemistry (2007), 18(2), 597-600

CODEN: BCCHES; ISSN: 1043-1802

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 146:478087

AB Simple synthesis of luminescent europium(III) and terbium(III) chelates tethered to a maleimido function is described. The method is based on the following: (i) synthesis of protected ligands tethered to a maleimido function and their purification on silica gel; (ii) deprotection by acidolysis; (iii) conversion of the deprotected ligands to the corresponding lanthanide(III) chelates by passing them through a column of strong cation exchange resin loaded with the appropriate lanthanide(III) ions.

According to this procedure, large quantities of mercapto-selective

biomol.-labeling reactants of high purity can be prepared

IT 189805-30-9

RL: RCT (Reactant); RACT (Reactant or reagent) (convenient synthesis of maleimido-derivatized lanthanide(III) chelates and their use in mercapto group conjugation)

RN 189805-30-9 CAPLUS

CN Glycine, N,N'-[[4-[2-(4-aminophenyl)ethyl]-H-pyrazole-1,3-diyl]bis(6,2-pyridinedlylmethylene)]bis[N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-, 1,1'-bis(1,1-dimethylethyl) ester (CA INDEX NAME)

IT 935687-82-4P 935687-84-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(convenient synthesis of maleimido-derivatized lanthanide(III) chelates and their use in mercapto group conjugation)

RN 935687-82-4 CAPLUS

CM

Glycine, N, N'=[{4-[2-[4-[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-y1)-1-oxohexyl]amino]phenyl]ethyl]-1H-pyrazole-1,3-diyl]bis(6,2-pyridinediy|methylene)]bis[N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-,1,1'-bis(1,1-dimethylethyl) ester (CA INDEX NAME)

PAGE 2-A

RN 935687-84-6 CAPLUS
CN Glycine, N,N'-[[4-[2-[4-[[6-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxohexyl]amino]phenyl]ethyl]-1H-pyrazole-1,3-diyl]bis(6,2-pyridinediylmethylene)]bis(N-(carboxymethyl)- (CA INDEX NAME)

PAGE 2-A

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

DOCUMENT NUMBER: 145:29304

2006:887897 CAPLUS 145:293047

TITLE: Preparation of heterocyclic compounds as activators

for peroxisome proliferator activated receptor δ
INVENTOR(S): Sakuma, Shogo; Mochiduki, Nobutaka; Takahashi, Rie;
Hirai, Toshitake; Yamakawa, Tomic; Masui, Selichiro

PATENT ASSIGNEE(S): Nippon Chemiphar Co., Ltd., Japan

SOURCE: PCT Int. Appl., 115pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

ACCESSION NUMBER:

PA:	TENT	NO.			KIN	D	DATE			APPI	ICAT	ION :	NO.		D	ATE	
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WO	2006	0909	20		A1		2006	0831		WO 2	006-	JP30	4193		2	0060	228
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	W: AE, AG, AL CN, CO, CR					CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,

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             MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
             SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
             VN, YU, ZA, ZM, ZW
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             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
     AU 2006217682
                          Α1
                                20060831
                                            AU 2006-217682
                                                                    20060228
     CA 2599454
                                20060831
                                            CA 2006-2599454
                                                                    20060228
                          A1
                                            EP 2006-715252
     EP 1854784
                          A1
                                20071114
                                                                    20060228
         R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL,
             BA, HR, MK, YU
     MX 200710511
                                20071107
                                            MX 2007-10511
                                                                    20070828
                          Α
     NO 2007004738
                                20071108
                                            NO 2007-4738
                                                                    20070917
                          Α
     KR 2007113253
                                            KR 2007-721867
                                                                    20070921
                          Α
                                20071128
     IN 2007CN04285
                          Α
                                20071221
                                            IN 2007-CN4285
                                                                    20070927
                                            CN 2006-80014554
     CN 101166720
                          Α
                                20080423
                                                                    20071029
PRIORITY APPLN. INFO.:
                                            JP 2005-52762
                                                                 A 20050228
                                            WO 2006-JP304193
                                                                   20060228
                                            WO 2006-JP4193
                                                                W 20060228
OTHER SOURCE(S):
                        MARPAT 145:293047
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AB The title compds. I [R1, R4 = H, alkyl, alkenyl, etc.; R2 = H; R3 = alkyl; or CR2R3 is CO, or CR2R3 is C=CR7R8; R7, R8 = H, alkyl; R5, R6 = H, alkyl, haloalkyl; X, Y = CH, N; Z = O, S; A = (un)substituted pyrazole, thiophene, furan, or pyrrole ring; B = (un)substituted alkylene; n = 0 - 5) are prepared Thus, 2-[4-{3-[3-isopropyl-1-(4-trifluoromethylphenyl)-1H-pyrazol-4-yl]propionyl]-2-methylphenoxy]-2-methylpropionic acid was prepared in a multistep process from [3-isopropyl-1-(4-trifluoromethylphenyl)-1H-pyrazol-4-yl]methanol. In an assay for the activation of peroxisome proliferator-activated receptor δ, compds. of this invention showed high activity.

Т

IT 908250-33-9P 908250-35-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclic compds. as activators for peroxisome proliferator-activated receptor δ)

RN 908250-33-9 CAPLUS

CN

Propanoic acid, 2-methyl-2-[2-methyl-4-[3-[3-(1-methylethyl)-1-(5-methyl-2-pyridinyl)-1H-pyrazol-4-yl]-1-oxopropyl]phenoxy]- (CA INDEX NAME)

PAGE 2-A

RN 908250-35-1 CAPLUS

CN Acetic acid, 2-[2-methyl-4-[3-[3-(1-methylethyl)-1-(5-methyl-2-pyridinyl)-1H-pyrazol-4-yl]-1-oxopropyl]phenoxy]- (CA INDEX NAME)

PAGE 2-A

HO2C-CH2-O

908250-30-6P 908250-32-8P 908250-34-0P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heterocyclic compds. as activators for peroxisome proliferator-activated receptor δ)

908250-30-6 CAPLUS

RN 1-Propanone, 1-(4-hydroxy-3-methylphenyl)-3-[3-(1-methylethyl)-1-(5-methyl-CN 2-pyridinyl)-1H-pyrazol-4-yl]- (CA INDEX NAME)

PAGE 2-A

908250-32-8 CAPLUS RN

Propanoic acid, 2-methyl-2-[2-methyl-4-[3-[3-(1-methylethyl)-1-(5-methyl-2-pyridinyl)-1H-pyrazol-4-yl]-1-oxopropyl]phenoxy]-, ethyl ester (CA INDEX NAME) CN

PAGE 2-A



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RN 908250-34-0 CAPLUS

CN Acetic acid, 2-[2-methyl-4-[3-[3-(1-methylethyl)-1-(5-methyl-2-pyridinyl)-1H-pyrazol-4-yl]-1-oxopropyl]phenoxy]-, ethyl ester (CA INDEX NAME)

PAGE 2-A

EtO-C-CH2-0

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS

L4 ANSWER 12 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

21

ACCESSION NUMBER: DOCUMENT NUMBER:

REFERENCE COUNT:

2006:884750 CAPLUS

145:293082 TITLE:

Preparation of pyrazolyl substituted xanthines as antagonists of A2B receptors

INVENTOR(S): Wang, Guoquan; Rieger, Jayson M.; Thompson, Robert D. PATENT ASSIGNEE(S): Adenosine Therapeutics, LLC, USA

SOURCE: PCT Int. Appl., 70pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PF	ATE	T	NO.			KIN	D	DATE			APPL	ICAT	I NOI	NO.		D.	ATE	
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WC	2	006	0918	97		A2		2006	0831		WO 2	006-	US67	46		2	0060	227
WC	2	006	0918	97		A3		2007	0222									
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			CN.	CO.	CR.	CII.	CZ.	DE.	DK.	DM.	DZ.	EC.	EE.	EG.	ES.	FT.	GB.	GD.

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GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM US 20070249598 A1 20071025 US 2006-362392 20060227 PRIORITY APPLN. INFO.: US 2005-656086P P 20050225 OTHER SOURCE(S): CASREACT 145:293082; MARPAT 145:293082

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AB Title compds. represented by the formula I [wherein R = H, (halo)alkyl, cycloalkyl, etc.; R1, R2 = independently H, (cyclo)alkyl, alkenyl, etc.; L1 = (un)substituted C, N, O, S or P, with proviso; Z = (un)substituted heteroaryl; Z1 = (un) substituted (hetero) aryl; n = 0-2; and pharmaceutically acceptable salts thereof] were prepared as A2B adenosine receptor (ARs) antagonists (no data). For example, cyclization of 6-chloronicotinoyl chloride with 5,6-diamino-1,3-dipropyluracil, and followed by reaction with hydrazine in EtOH, gave 1,3-dipropy1-8-(6-hydrazino-3-pyridy1)xanthine. I were tested for affinity with A2B receptors in HEK-293 cells. Thus, I and their pharmaceutical compns. are useful as A2B adenosine receptors antagonists for the treatment of A2B receptors mediated diseases, such as asthma, allergy immune disease, and etc. IΤ 908241-89-4P 908241-90-7P 908241-91-8P

908241-99-4P 908241-90-7P 908241-91-9P RL: PRC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (USes)

(preparation of pyrazolyl substituted xanthines as antagonists of A2B receptors)

RN 908241-89-4 CAPLUS CN 1H-Puripe-2.6-dione

1H-Purine-2,6-dione, 1-cyclopropy1-3,9-dihydro-8-[6-(4-phenyl-1H-pyrazol-1-yl)-3-pyridinyl]-3-propyl- (CA INDEX NAME)

RN 908241-90-7 CAPLUS

CN 1H-Purine-2,6-dione, 1-cyclopropyl-3,9-dihydro-8-[6-[4-(4-methoxyphenyl)-1H-pyrazol-1-yl]-3-pyridinyl]-3-propyl- (CA INDEX NAME)

RN 908241-91-8 CAPLUS

CN 1H-Purine-2,6-dione, 1-cyclopropyl-3,9-dihydro-3-propyl-8-[6-[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]-3-pyridinyl]- (CA INDEX NAME)

L4 ANSWER 13 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:693655 CAPLUS

DOCUMENT NUMBER: 145:167214

TITLE: Antibacterial and antifungal activities of new pyrazolo[3,4-d]pyridazine derivatives. [Erratum to

document cited in CA143:007682]

AUTHOR(S): Akbas, Esvet; Berber, Ismet CORPORATE SOURCE: Organic Chemistry Division.

Organic Chemistry Division, Chemistry Department,

Faculty of Arts and Sciences, Yuzuncu Yil University, Van, 65080, Turk.

SOURCE: European Journal of Medicinal Chemistry (2006), 41(7),

CODEN: EJMCA5; ISSN: 0223-5234

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

On page 401, Abstract line 1 and Introduction line 23 and 24, the word "new" AB before "1H-pyrazole-3-carboxylic acids" should be omitted. Abstract should read: "Several new pyrazolo[3,4-d]pyrazole-3-carboxylic acids and various hydrazines.". Introduction should read: "As the results of these reactions were synthesized pyrazole-3-carboxylic acids [12,13]. The acids were converted into various derivs. of the pyrazole-pyridazine with different hydrazines.". On page 402, left column, starting with line 1 the text should read: "The compound 3 can easily be transformed into the corresponding acid chloride 4 and amide 5 derivs. [12] by the usual chemical procedures. Furthermore, a cold solution of the acid amide 5 in a mixture of DMF and SOC12 was stirred at 0-5 °C for 2 h to give nitrile 6 [12] (Scheme 2) (see exptl. for details).". Refs. 12 and 13 should be added. Reference 12 should read: "E. Akbas, I. Berber, A. Sener, B. Hasanov II, Farmaco 60 (2005) 23-26.". Reference 13 should read: "A. Sener, E. Akbas, M.K. Sener, Turkish Journal of Chemical 28 (2004) 271-277.". 791112-66-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, antibacterial, and antifungal activity of of pyrazolopyridazine derivs. starting from benzovl(phenyl)furandione and hydrazines using cyclization as the key step (Erratum))

RN 791112-66-8 CAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 4-benzoyl-5-phenyl-1-(2-pyridinyl)- (CA INDEX NAME)

ANSWER 14 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

2006:386429 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 144:432797

TITLE: Preparation of diaryl substituted pyrazoles and

analogs for nonsense suppression

INVENTOR(S): Almstead, Neil; Karp, Gary M.; Wilde, Richard; Welch,

Ellen; Campbell, Jeffrey A.; Ren, Hongyu; Chen,

Guangming

PTC Therapeutics, Inc., USA PATENT ASSIGNEE(S): SOURCE:

PCT Int. Appl., 286 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PA'	TENT	NO.			KIN	D	DATE			APPL	ICAT	ION :	NO.		D.	ATE	
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WO	2006	0445	02		A2		2006	0427		WO 2	005-	US36	761		2	0051	013
WO	2006		A3		2006	0803											
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            YU, ZA, ZM, ZW
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            CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG, BW, GH,
            GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM
    AU 2005295727
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PRIORITY APPLN. INFO.:
                                           US 2004-617633P
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                                           US 2004-617634P
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                                           US 2004-617653P
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                                           US 2004-617655P
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                                           US 2004-617670P
                                                             P 20041013
                                                            P 20041103
W 20051013
                                           US 2004-624170P
                                           WO 2005-US36673
                                           WO 2005-US36761 W 20051013
OTHER SOURCE(S):
                    MARPAT 144:432797
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R2 Ar4
Ar2
Ar3
Ar1

GΙ

AB The present invention relates to methods, compds., and compns. for treating or preventing diseases associated with nonsense mutations in an mRNA by administering the compds. I (Al = C, CH, or N; V and X = N or C; W = N, C or CH; wherein at least one of V, W, or X = N, and wherein if W = N, at least one of V or X is also N; Y and Z = N, CRa, CO, CS (Ra = H, Me, NHZ); R1 = carboxy, cyano, or carbonyl which is optionally substituted with alkoxy, R2 = absent or nitro; Arl = (un)substituted alkyl, aryl, 5-10

membered heterocyclyl; or Arl together with Ar2 form a ring; or Arl together with Ar3 form a ring; Ar2 is absent or together with Ar1 form a ring; Ar3 is absent or together with Ar1 form a ring; Ar3 is absent or together with Ar1 form a ring; Ar4 is absent or is alkyl, alkoxy, thioalkyl, any of which together with Al forms a 4-7 membered carbocycle or heterocycle] or compns. comprising I. More particularly, the present invention relates to methods, compds., and compns. for suppressing premature translation termination associated with a nonsense mutation in an mRNA. Over 470 compds. I were prepared E.g., a multi-step synthesis of 3-[1-(4-trifloromethylphenyl)-IR-pyrrol-3-yl)benzoic acid, starting from 1-(trifsopropylsilyl)pyrrole-3-boronic acid and Me 4-iodobenzoate, was given. Compds. I were tested for nonsense suppression activity from a cell-based luciferase reporter assay (data given).

IT 885016-97-7P 885016-98-8P 885017-23-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of diaryl pyrazoles and analogs for suppressing premature translation termination associated with nonsense mutation in an mRNA and useful in treating and preventing diseases-associated with nonsense mutations in an mRNA)

RN 885016-97-7 CAPLUS

CN Benzoic acid, 3-[1-(2-pyridinyl)-1H-pyrazol-4-yl]- (CA INDEX NAME)

RN 885016-98-8 CAPLUS

CN Benzoic acid, 4-[1-(2-pyridinyl)-1H-pyrazol-4-yl]- (CA INDEX NAME)

885017-23-2 CAPLUS RN

CMBenzoic acid, 3-[1-[5-(trifluoromethyl)-2-pyridinyl]-1H-pyrazol-4-yl]-(CA INDEX NAME)

ANSWER 15 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN 2006:169674 CAPLUS

ACCESSION NUMBER:

DOCUMENT NUMBER: 144:412415

TITLE: Synthesis, Pharmacology, and Structure-Activity

Relationships of Novel Imidazolones and Pyrrolones as

Modulators of GABAA Receptors Grunwald, Christian; Rundfeldt, Chris; Lankau, AUTHOR(S):

Hans-Joachim; Arnold, Thomas; Hoefgen, Norbert; Dost,

Rita; Egerland, Ute; Hofmann, Hans-Joerg; Unverferth, Klaus

CORPORATE SOURCE: elbion AG, Radebeul, D-01445, Germany

SOURCE: Journal of Medicinal Chemistry (2006), 49(6), 1855-1866

CODEN: JMCMAR; ISSN: 0022-2623

American Chemical Society PUBLISHER:

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:412415 AB New series of imidazolones and pyrrolones were synthesized. The compds. were tested for their anxiolytic properties due to modulation of the GABAA receptor response. Several derivs. exhibit considerable pharmacol. activity while lacking the typical side effects of benzodiazepine receptor agonists. 1-(4-Chlorophenyl)-4-morpholin-1-yl-1,5-dihydro-imidazol-2-one and 1-(4-chlorophenyl)-4-piperidin-1-y1-1,5-dihydro-imidazo1-2-one were protective in the pentylenetetrazole test in rats with oral ED50 of 27.4 and 12.8 mg/kg and TD50 (rotarod) of >500 and 265 mg/kg, resp. The min. ED in the Vogel conflict test was 3 mg/kg for both compds. Common structure-activity relationship and comparative mol. field anal. models of the various series of derivs. could be established which are in accordance with a GABAA mediated pharmacol. action. The findings fit well into an established pharmacophore model. This model is refined by an addnl. steric restriction feature.

883943-17-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of amino(aryl)imidazoles and -pyrroles as GABAA receptor

agonists)

883943-17-7 CAPLUS RN

CN Pyridine, 2-[4-(4-chlorophenyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)



REFERENCE COUNT: 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:

2006:164594 CAPLUS 144:254143

DOCUMENT NUMBER:

INVENTOR(S):

Preparation of 2-cyanopyrimidine derivatives as TITLE: cathepsin S inhibitors for treatment of neuropathic

Hart, Terance William; Hallett, Allan; Yokokawa,

Fumiaki; Hirao, Hajime; Ehara, Takeru; Iwasaki,

Atsuko; Sakaki, Junichi; Masuya, Keiichi; Kishida, Masashi; Irie, Osamu

PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.

SOURCE: PCT Int. Appl., 111 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE: FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.					KIND DATE				APPL			DATE						
	2006				A1 20060223			WO 2005-EP8896						20050816					
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,		
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		LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,		
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AU 2005274319				A1		2006	0223	- 1	AU 2	005-	2743	19		2	0050	816			
CA	2575	826			A1					CA 2	CA 2005-2575826						20050816		

EP	1781	623			A1 20070509					EΡ	20	05-	7824	60	20050816			
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		IS,	IT,	LI,	LT,	LU,	LV,	MC,	NL,	PΙ	٠,	PT,	RO,	SE,	SI,	SK,	TR	
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JP	2008	5099	59		T		2008	0403		JP	20	07-	5263	82		2	0050	816
BR	2005	0143	83		A		2008	0610		BR	20	05-	1438	3		2	0050	816
IN	2007	DN01	085		A		2007	0803		IN	20	07-1	DN10	85		2	0070	208
KR	2007	0361	83		A		2007	0402		KR	20	07-	7039	02		2	0070	216
MX	2007	0195	2		A		2007	0509		MX	20	07-	1952			2	0070	216
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										WO	20	05-1	EP88	96	1	W 2	0050	816
OTHER SO	URCE	(S):			MARE	PAT	144:	2541	13									

TT

- AB The title 2-cyanopyrimidine derivs. I [wherein R1 = (cycloalkyl)alkyl, (bicycloalkyl)alkyl, etc.; R2 = halo, alkyl, (un)substituted aryl, etc.; R3 = H, halo, (un)substituted Ph, pyridyl, etc.; X = O, NH, S, etc.], or tautomers, or salts thereof were prepared For example, the compound II was prepared in a multi-step synthesis. I are useful as inhibitors of cathepsin S for the treatment of neuropathic pain (no data). A formulation containing I as an active ingredient was also described. ΙT 877125-72-9P
 - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of 2-cyanopyrimidine derivs. as cathepsin S inhibitors for treatment of neuropathic pain)

- RN 877125-72-9 CAPLUS
- CN 1H-Pyrazol-5-amine, 4-phenyl-1-(2-pyridinyl)- (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT ACCESSION NUMBER: 2005:1354392 CAPLUS

DOCUMENT NUMBER: 144:88317

TITLE: Preparation of heterocycle-containing alkynyl derivatives as modulators of metabotropic glutamate

receptors

INVENTOR(S): Bessis, Anne-Sophie; Bolea, Christelle; Bonnet,

Beatrice; Epping-Jordan, Mark; Poirier, Nicholas; Poli, Sonia-Maria; Rocher, Jean-Philippe; Thollon,

Yves

PATENT ASSIGNEE(S): Addex Pharmaceuticals SA, Switz.

SOURCE: PCT Int. Appl., 308 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.		APPLICATION NO.	
	A2 20051229	WO 2005-IB2390	
W: AE, AG, AI CN, CO, CI GE, GH, GR LC, LK, LI NG, NI, N SL, SM, S3 ZA, ZM, Zi RN: BW, GH, GR AZ, BY, KC EE, ES, F1	, AM, AT, AU, AZ, CU, CZ, DE, DK, HR, HU, ID, IL, LS, LT, LU, LV, NZ, OM, PG, PH, TJ, TM, TN, TR, KE, LS, MW, MZ, KZ, MD, RU, TJ, FR, GB, GR, HU,	BA, BB, BG, BR, BW, DM, DZ, EC, EE, EG, IN, IS, JP, KE, KG, IN, IS, JP, KE, KG, MA, MD, MG, MK, MN, PL, PT, RO, RU, SC, TT, TZ, UA, UG, US, NA, SD, SL, SZ, TZ, TM, AT, BE, BG, CH, IE, IS, IT, LT, LU,	ES, FI, GB, GD, KM, KP, KR, KZ, MW, MX, MZ, NA, SD, SE, SG, SK, UZ, VC, VN, YU, UG, ZM, ZW, AM, CY, CZ, DE, DK, MC, NL, PL, PT,
MR. NE. SI	, TD, TG	CF, CG, CI, CM, GA,	, , ,
CA 25/0987 EP 1765795 R: AT, BE, BE, BE IS, IT, LI HR, LV, MI CN 101001846 BR 2005011072 JP 2008502674 MX 2006EPA14721 IN 2006CN04639 KR 2007054624	A1 20051229 A2 20070328 , CH, CY, CZ, DE, , LT, LU, MC, NL, , YU A 20070127 T 20080131 A 20070629 A 20070629 A 200701529 A 200701529	AU 2005-254808 CA 2005-2570987 EP 2005-766895 DK, EE, ES, FI, FR, PL, PT, RO, SE, SI, CN 2005-80026025 BR 2005-11072 JP 2007-516076 MX 2006-PA14721 IN 2006-CM4639 KR 2007-2088 GB 2004-13605	20050617 20050617 GB, GR, HU, IE, SK, TR, AL, BA, 20050617 20050617 20050617 20061214 20061218 20070112
OTHER SOURCE(S):		WO 2005-IB2390	W 20050617

$$C \equiv C$$

- AB The present invention relates to heterocycle-containing alkynyl derivs. (WC.tplbond.C(CH2)nXW' (I); variables defined below; e.g. 1-methyl-2-[4-(pyridin-2-yl)-3-butynyl]-1H-benzo[d]imidazole (shown as II)) that are modulators of metabotropic glutamate receptors - subtype 5 ("mGluR5") and are therefore useful for the treatment of central nervous system disorders as well as other disorders modulated by mGluR5 receptors. Methods of preparation are claimed and prepns, and/or characterization data for .apprx.250 examples of I are included. For example, II was prepared in 4 steps (not stated, 23, 70 and 31 % yields, resp.) starting with chlorination of (1-methyl-1H-benzimidazol-2-yl)methanol to give 2-chloromethyl-1-methyl-1H-benzimidazole, which was coupled with trimethylprop-1-ynylsilane to give 1-methyl-2-[4-(trimethylsilanyl)-3-butynyl]-1H-benzimidazole, which was deprotected to give 2-(3-butynyl)-1-methyl-1H-benzimidazole, which was coupled with 2-iodopyridine to give II. For I: W is a 5-, 6-heterocyclic ring containing a N adjacent to the ethynyl bond, which ring may optionally be fused with a 5- or 6-membered ring containing ≥1 atoms independently C, N, O and S; X = an (un)substituted C1-C6-alkyl, C1-C6-alkylhalo, C2-C6-alkynyl, C2-C6-alkenyl, O-C0-C6-alkyl, O-C1-C6-alkylhalo, O-C3-C6-alkynvl, O-C3-C6-alkenvl, O-C3-C7-cvcloalkvl, C1-C6-alkvl-O, C3-C7-cvcloalkvl, C3-C7-cvcloalkvl-C0-C6-alkvl, et al.; W' = a 5- or 6-membered ring containing ≥1 atoms = C, N, O and S, which ring may optionally be fused with a 5- or 6-membered ring containing ≥1 atoms = C, N, O and S; addnl. details including provisos are given in the claims. Results of a mGluR5 binding assay for >200 examples of I are tabulated; also test results of a marble burying model of anxiety in mice and Vogel conflict drinking model of anxiety in rats are discussed. 872365-27-0P, 2-[4-(4-Phenyl-1H-pyrazol-1-y1)-1-butynyl]pyridine 872366-02-4P, 2-[4-[4-(4-Fluorophenyl)-1H-pyrazol-1-yl]-1butynyl]pyridine 872366-09-1P, 2-[4-(4-(0-Tolyl)-1H-pyrazol-1-yl]-1-butynyl]pyridine 872366-15-9P
 - 2-(Fluoromethyl)-6-[4-[4-(o-tolyl)-1H-pyrazol-1-yl]-1-butynyl]pyridine

872366-17-1P, 2-(Fluoromethyl)-6-[4-[4-(4-fluorophenyl)-1H-pyrazol-1-y1]-1-butynyl]pyridine 872367-17-4P, 2-[4-(3-Methyl-4-phenyl-1H-pyrazol-1-yl)-1-butynyl]pyridine

872367-18-5P, 2-[4-(5-Methyl-4-phenyl-1H-pyrazol-1-yl)-1-

butynyl]pyridine RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of heterocycle-containing alkynyl derivs. as modulators of metabotropic glutamate receptors)

RN 872365-27-0 CAPLUS

CN Pyridine, 2-[4-(4-phenyl-1H-pyrazol-1-yl)-1-butyn-1-yl]- (CA INDEX NAME)

$$N$$
 N CH_2 CH_2 C C N

RN 872366-02-4 CAPLUS

CN Pyridine, 2-[4-[4-(4-fluoropheny1)-1H-pyrazo1-1-y1]-1-butyn-1-y1]- (CA INDEX NAME)

RN 872366-09-1 CAPLUS

CN Pyridine, 2-[4-[4-(2-methylphenyl)-1H-pyrazol-1-yl]-1-butyn-1-yl]- (CA INDEX NAME)

Me

RN 872366-15-9 CAPLUS

CN Pyridine, 2-(fluoromethy1)-6-[4-[4-(2-methylphenyl)-1H-pyrazol-1-yl]-1-butyn-1-yl]- (CA INDEX NAME)

$$\label{eq:NNN} \text{N---} \text{CH}_2\text{---} \text{CH}_2\text{---} \text{C} = \text{C} - \text{N}$$
 Me
$$\text{CH}_2\text{F}$$

RN 872366-17-1 CAPLUS

CN Pyridine, 2-(fluoromethyl)-6-[4-[4-(4-fluorophenyl)-1H-pyrazol-1-yl]-1butyn-1-yl]- (CA INDEX NAME)

RN 872367-17-4 CAPLUS

Pyridine, 2-[4-(3-methyl-4-phenyl-1H-pyrazol-1-yl)-1-butyn-1-yl]- (CA CN INDEX NAME)

Me N
$$CH_2-CH_2-C = C$$
 N Ph

RN 872367-18-5 CAPLUS

CN Pyridine, 2-[4-(5-methyl-4-phenyl-1H-pyrazol-1-yl)-1-butyn-1-yl]- (CA INDEX NAME)

L4 ANSWER 18 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1289898 CAPLUS

DOCUMENT NUMBER: 144:36334

TITLE: Preparation of phenyl benzovl pyrazoles as CRTH2

receptor ligands INVENTOR(S):

Ulven, Trond; Frimurer, Thomas; Rist, Oeystein;

Kostenis, Evi; Hoegberg, Thomas; Receveur, Jean-Marie; Grimstrup, Marie

PATENT ASSIGNEE(S): 7TM Pharma A/S, Den.

SOURCE: PCT Int. Appl., 115 pp.

CODEN: PIXXD2 Patent

DOCUMENT TYPE: LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.					KIND DATE				APPLICATION NO.						DATE			
	2005				A1		2005	1208	WO 2005-EP5884									
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,	
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KM,	KP,	KR,	KZ,	
		LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	
		NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	
		SL,	SM,	SY,	TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	
		ZA,	ZM,	ZW														
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	
		AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT,	
		RO,	SE,	SI,	SK,	TR,	BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	
		MR,	NE,	SN,	TD,	TG												
ΑU	2005	2471	10		A1	20051208			AU 2005-247110						20050530			
CA	2568	766			A1		20051208			CA 2005-2568766					20050530			

EP	17585	A1		2007	0307		EΡ	200	05-	7702	20		20050530					
	R:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EF	E, 1	ES,	FI,	FR,	GB,	GR,	HU,	IE,
		IS,	IT,	LI,	LT,	LU,	MC,	NL,	PL,	P1	Γ, Ι	RO,	SE,	SI,	SK,	TR,	AL,	BA,
		HR,	LV,	MK,	YU													
CN	19806	64			A		2007	0613		CN	200	05-	8002	2625		2	0050	530
BR	20050	116	76		A		2008	0108		BR	200	05-	1167	6		2	0050	530
JP	20085	5009	91		T		2008	0117		JP	200	07-	5138	46		2	0050	530
MX	2006E	A13	912		A		2007	0718		MX	200	06-1	PA13	912		2	0061	129
NO	20060	060	48		A		2007	0227		ИО	200	06-	6048			2	0061	228
KR	20070	451	53		A		2007	0502		KR	200	06-	7275	04		2	0061	228
IN	20060	CNO4	778		A		2007	0629		ΙN	200	06-0	CN47	78		2	0061	228
PRIORIT	Y APPI	N.	INFO	. :						GB	200	04-	1219	8		A 2	0040	529
										GB	200	04-	1419	6		A 2	0040	624
										GB	200	04-	2401	8		A 2	0041	029
										WO	200	05-1	EP58	84		W 2	0050	530
OWNED OF	OUTDON.				143.00	2. m	2 4 4 -	2022	4									

OTHER SOURCE(S): MARPAT 144:36334 GI

Ar2-L2-Ar1-L3-(Ar3)nH I

AB Title compds. I [A = carboxy, carboxy bioisostere; Al = H, Me; Arl = (un)substituted heteroaryl in which the groups CGHAN and L2 are linked to adjacent ring atoms; Ar2-3 = heteroaryl; n = 0-1; L2-3 = divalent radical (Alk1)m-Zq-(Alk2)p; m, q, p = 0-1; Alk1-2 = alkylene which may be heteroatom substituted, etc.; Z = 0, S, CO SO2, etc.; with some provisions] are prepared For instance, 4-bromo-2-((1-phenyl-IH-pyrazole-4-yl)carbonyl)phenoxyacetic acid (II) is prepared in 2 steps from (5-bromo-2-hydroxyphenyl)(1-phenyl-IH-pyrazol-4-yl)methanone and Et bromoacetate. II has an ICSO < 0.5 µM for the CRTM2 receptor. I are useful for the treatment of disease responsive to modulation of CRTM2 receptor activity, such as asthma, thinitis, alleroic

airway syndrome, and allergic rhinobronchitis.

IT 870809-77-IP

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(preparation of Ph benzoyl pyrazoles as CRTH2 receptor ligands)

RN 870809-77-1 CAPLUS

CN Acetic acid, 2-[4-bromo-2-[[1-(2-pyridinyl)-1H-pyrazol-4yl]carbonyl]phenoxy]- (CA INDEX NAME) 10/551,709

- IT 870811-23-7P 870811-31-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of Ph benzoyl pyrazoles as CRTH2 receptor ligands)
- RN 870811-23-7 CAPLUS
- CN Methanone, (5-bromo-2-hydroxyphenyl)[1-(2-pyridinyl)-1H-pyrazol-4-yl]-(CA INDEX NAME)

- RN 870811-31-7 CAPLUS
- CN Acetic acid, 2=[4-bromo-2-[[1-(2-pyridinyl)-1H-pyrazol-4-yl]carbonyl]phenoxy]-, ethyl ester (CA INDEX NAME)

REFERENCE COUNT:

6 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:376646 CAPLUS

DOCUMENT NUMBER: 143:43822

TITLE: Palladium-catalyzed coupling of pyrazoles with

2,6-dibromopyridine

AUTHOR(S): Sun, Xiaojiao; Yu, Zhengkun; Deng, Haixia; Wu,

Xiaowei; Wu, Sizhong; Dong, Jinhua CORPORATE SOURCE: Dalian Institute of Chemical Physics, The Chinese

Academy of Sciences, Dalian, Liaoning, 116023, Peop.

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS

Rep. China

SOURCE: Cuihua Xuebao (2005), 26(3), 173-174 CODEN: THHPD3; ISSN: 0253-9837

PUBLISHER: Kexue Chubanshe

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:43822

A number of 1H-pyrazoles (substitution patterns: H, 3-Me, 3,5-Me2, 3,4,5-Me3, 3,5-Me2-4-Bn, 3-Me-5-Ph, 3,5-Ph2, and 3,5-tert-Bu2) were reacted with 2.6-dibromopyridine and the ratio of mono- and disubstituted pyrazolylpyridines was determined in presence and absence of the Pd(OAc)2/PPh3 catalyst and in dependence of molar ratio of reactants (1:1 and 1:2.4 pyridine/pyrazole). While the 3,5-tert-Bu2-substituted pyrazole did not react al all, the other pyrazoles formed the pyrazolylpyridines with broad varying yields and with nearly exclusive formation of the mono-substituted products when the reactants are used in equimolar ratio. When pyrazoles are used in excess, mono- and disubstituted products were obtained. The use of catalyst often lowered yield and shifted product ratio to

mono-substitution when pyrazoles are used in excess (exception: unsubstituted pyrazole).

853748-43-3P 853748-47-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (palladium-catalyzed coupling of pyrazoles with 2,6-dibromopyridine for

preparation of mono- and dipyrazolyl-substituted pyridine derivs.) RN 853748-43-3 CAPLUS

CN Pyridine, 2-bromo-6-[3,5-dimethyl-4-(phenylmethyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)

RN 853748-47-7 CAPLUS

CN Pyridine, 2,6-bis[3,5-dimethyl-4-(phenylmethyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 20 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:371577 CAPLUS

DOCUMENT NUMBER: 143:43821

TITLE: Base Effect and Inhibition of Catalytic Activity in Palladium-Catalyzed N-Heteroarylation of Pyrazoles

with 2,6-Dibromopyridine

AUTHOR(S): Sun, Xiaojiao; Yu, Zhengkun; Wu, Sizhong; Wen, Jing CORPORATE SOURCE: Dalian Institute of Chemical Physics, Chinese Academy

of Sciences, Liaoning, 116023, Peop. Rep. China

SOURCE: Organometallics (2005), 24(12), 2959-2963

CODEN: ORGND7; ISSN: 0276-7333

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE:

English

CASREACT 143:43821 OTHER SOURCE(S):

2,6-Bis(1-pyrazoly1)pyridines were prepared by palladium-catalyzed coupling of pyrazoles with 2,6-dibromopyridine. 3-R1-4-R2-5-R3-Pyrazoles (2a-h; R1, R2, R3: a H, H, H; b H, H, Me; c Me, H, Me; d Me, Me, Me; e Me, CH2Ph, Me; f Ph, H, Me; g Ph, H, Ph; h tBu, H, tBu) undergo coupling with 2,6-dibromopyridine (1) in the presence of Pd(OAc)2/PPh3 catalyst and KOtBu or NaOtBu as a base. The reaction in a molar ratio of 1:2:base = 1:2.4:2.5 afforded the monosubstituted products 2-bromo-6-(3-R1-4-R2-5-R3-1H-pyrazol-1-yl)pyridines (3a-g) as the major products when KOtBu was used as the base, together with 69-30% of the disubstituted 2,6-bis(3-R1-4-R2-5-R3-1H-pyrazol-1-y1)pyridines (4a-f, same Rn). Without using the catalyst or using NaOtBu as the base the disubstituted compds. 4a-f were formed as the major products in yields up to 93%. Reactions of 1 and 2 in a molar ratio of 1:2:base = 1:1:1

selectively produced compds. 3 in yields up to 82% when KOtBu was used as the base. The complex from the reaction of 3 and Pd(OAc)2 did not undergo further reaction with 1 to form 4 in the presence of a base. The base effect and inhibition of catalytic activity for Pd(OAc)2 are discussed.

853748-43-3P 853748-47-7P RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of substituted 2-pyrazolyl- and 2,6-dipyrazolylpyridines by palladium-catalyzed coupling of 2.6-dibromopyridine with pyrazoles)

RN 853748-43-3 CAPLUS

CN Pyridine, 2-bromo-6-[3,5-dimethyl-4-(phenylmethyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)

RN 853748-47-7 CAPLUS

CN Pyridine, 2,6-bis[3,5-dimethyl-4-(phenylmethyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

32 L4 ANSWER 21 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:331854 CAPLUS DOCUMENT NUMBER:

143:7682

TITLE: Antibacterial and antifungal activities of new

pyrazolo[3, 4-d]pyridazine derivatives

AUTHOR(S): Akbas, Esvet; Berber, Ismet

Organic Chemistry Division, Chemistry Department, CORPORATE SOURCE:

Faculty of Arts and Sciences, Yuzuncu Yil University,

Van, 65080, Turk.

SOURCE: European Journal of Medicinal Chemistry (2005), 40(4), 401-405

CODEN: EJMCA5; ISSN: 0223-5234

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:7682 G1

AB Several pyrazolo[3,4-d]pyridazine derivs., e.g., I, were prepared by the reaction of two lM-pyrazole-3-carboxylic acids and various hydrazines. The compds. were tested for antimicrobial activities against Gram-neg., Gram-pos. bacteria and fungi. Two of the tested compds. showed excellent antimicrobial activities against Gram-neg., Gram-pos. bacteria and fungi with min. inhibitory concors. in the range of 0.31 to < 0.0024 mg mL-1.

IT 791112-66-8P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, antibacterial, and antifungal activity of of pyrazolopyridazine derivs. starting from benzoyl(phenyl)furandione and hydrazines using cyclization as the key step)
791112-66-8 CAPLUS

RN 791112-66-8 CAPLUS CN 1H-Pyrazole-3-carboxylic acid, 4-benzoyl-5-phenyl-1-(2-pyridinyl)- (CA INDEX NAME)

REFERENCE COUNT:

11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 22 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:29859 CAPLUS DOCUMENT NUMBER: 142:430215
TITLE: Transformations of

Transformations of 5-amino-4-(3,4-dimethoxyphenyl)pyrazoles in the diazotization reaction

AUTHOR(S): Pavlov, I. V.; Kobrakov, K. I.; Bogza, S. L.

CORPORATE SOURCE: A. N. Kosygin Moscow State Technical University,

Moscow, 119991, Russia

SOURCE: Chemistry of Heterocyclic Compounds (New York, NY,

United States) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2004), 40(7),

964-965

CODEN: CHCCAL; ISSN: 0009-3122

PUBLISHER: Kluwer Academic/Consultants Bureau

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:430215

AB Diazotization of 5-amino-3-(4-chlorophenyl)-1-(3,5-dichloropyridin-2-yl)-4(3,4-dimethoxyphenyl)pyrazole in AcOH afforded via intramol. azo coupling
the 1-(4-chlorophenyl)-3-(3,5-dichloropyridin-2-yl)-7,8-dimethoxy-3Hpyrazolo[3,4-c]cinnoline while diazotization in H2504 in the presence of
arenes (2-hydroxynaphthalene or N,N-dimethylaniline) resulted in the
formation of the corresponding 5-arylazo derivs. of the starting
aminopyrazole via intermol. azo coupling.

IT 851040-12-5

RL: RCT (Reactant); RACT (Reactant or reagent) (transformations of 5-amino-4-(3,4-dimethoxyphenyl)-1-(3,5-dichloropyridin-2-yl)pyrazoles by diazotization reaction to 3-(3,5-dichloropyridin-2-yl)-7,8-dimethoxy-3H-pyrazolo[3,4-c]cinnoline and 5-arylazo-aminopyrazole derive.)

RN 851040-12-5 CAPLUS

CN 1H-Pyrazol-5-amine, 3-(4-chlorophenyl)-1-(3,5-dichloro-2-pyridinyl)-4-(3,4-dimethoxyphenyl)- (CA INDEX NAME)

IT 851040-14-7P 851040-15-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (transformations of 5-amino-4-(3,4-dimethoxyphenyl)-1-(3,5-dichloropyridin-2-yl)pyrazoles by diazotization reaction to 3-(3,5-dichloropyridin-2-yl)-7,8-dimethoxy-3H-pyrazolo[3,4-c]cinnoline and 5-arylazo-aminopyrazole derivs.)

RN 851040-14-7 CAPLUS

CN 2-Naphthalenol, 1-[2-[3-(4-chlorophenyl)-1-(3,5-dichloro-2-pyridinyl)-4-(3,4-dimethoxyphenyl)-1H-pyrazol-5-yl]diazenyl]- (CA INDEX NAME)

RN 851040-15-8 CAPLUS

CN

Benzenamine, 4-[2-[3-(4-chlorophenyl)-1-(3,5-dichloro-2-pyridinyl)-4-(3,4dimethoxyphenyl)-1H-pyrazol-5-yl]diazenyl]-N,N-dimethyl- (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 23 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2004:878273 CAPLUS

3

DOCUMENT NUMBER: 141:366220

Preparation of diaryl substituted pyrazole modulators TITLE: of metabotropic glutamate receptor-5

INVENTOR(S): Cosford, Nicholas D. P.; Eastman, Brian W.; Huang,

Dehua; Smith, Nicholas D.; Tehrani, Lida R. PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Essa Hu

SOURCE: PCT Int. Appl., 72 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO.		DATE						
WO 2004089303				211661				
WO 2004089303				211021	20040550			
					DE 01 011			
W: AE, AG, AL								
			DM, DZ, EC, I					
			IN, IS, JP, I					
			MD, MG, MK, 1					
			RO, RU, SC, S					
			UG, US, UZ, Y					
RW: BW, GH, GM	KE, LS,	MW, MZ,	SD, SL, SZ, 3	rz, ug, zm,	ZW, AM, AZ,			
BY, KG, KZ	MD, RU,	TJ, TM,	AT, BE, BG, G	CH, CY, CZ,	DE, DK, EE,			
ES, FI, FR	GB, GR,	HU, IE,	IT, LU, MC, I	NL, PL, PT,	RO, SE, SI,			
SK, TR, BF	BJ, CF,	CG, CI,	CM, GA, GN, C	GQ, GW, ML,	MR, NE, SN,			
TD, TG								
AU 2004228057	A1 :	20041021	AU 2004-22	28057	20040330			
CA 2520870	A1 :	20041021	CA 2004-25	520870	20040330			
EP 1613614								
R: AT, BE, CH	DE. DK.	ES. FR.	GB. GR. IT. I	T. LIL NI.	SE. MC. PT.			
			CY, AL, TR, I					
CN 1795184								
JP 2006522164	т	20060928	JP 2006-51	10074	20040330			
IN 2005DN04191	Δ .	20070831	TN 2005-D	1/191	20010330			
US 20060194807	7.1	20070031	HC 2005 BI	1700	20051003			
PRIORITY APPLN. INFO.:		20000031			P 20030403			
PRIORITI APPLIN. INFO.:					W 20040330			
OTHER SOURCE(S):	MARPAT	141.36622		211021	w 20040330			
GI			-					

AB Title compds. represented by the formula I [wherein X, Y = independently (hetero)aryl, and at least one of X and Y is a heteroaryl with N adjacent to the position of attachment to A or B; A, B = independently (hetero)alkyl, alkylsulfonylalkyl, alkylcarbonylalkyl, etc.; W, Z = independently (un)substituted (hetero)cycloalkyl, alkyl(hetero)aryl; one of Al and A2 is N, the other in (un)substituted C; R1l = halo, alkyl, alkoy(ln) (in)(alkyl); and pharmaceutically acceptable salts thereof]

were prepared as modulators of metabotropic glutamate receptor-5 (mGluR5). For example, reaction of 2-(2-ppridyl) malondialdehyde with hydrazine hydrate (60%), followed by substitution with

1-bromo-3-chloro-5-fluorobenzene (45%) and coupling reaction with pyridin-3-ylboronic acid (80%), gave II. The prepared I were tested for mGGuR5 inhibitory activity with IC50 value of about 2 µM in the calcium flux assay. Thus, I and their pharmaceutical compns. are useful as modulators of mGluR5 for the treatment of panic, and bipolar disorder, as well as in the treatment of psychiatric and mood disorders such as, for example, schizophrenia, anxiety, depression, panic, and bipolar disorder, as well as in the treatment of pain, Parkinson's disease, cognitive dysfunction, epilepsy, circadian rhythm disorders, obesity, drug addiction, drug abuse, drug withdrawal and other diseases (no data).

IT 777880-83-8P 777881-01-3P 777881-25-1P 777881-29-5P 777881-33-1P 777881-94-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of diaryl pyrazole modulators of metabotropic glutamate receptor-5)

RN 777880-83-8 CAPLUS

CN Pyridine, 2-[4-[3-chloro-5-(3-pyridinyl)phenyl]-1H-pyrazol-1-yl]- (CA INDEX NAME)

RN 777881-01-3 CAPLUS

CN Pyridine, 2-[4-[3-methoxy-4-(2-pyridinyl)phenyl]-1H-pyrazol-1-yl]- (CA INDEX NAME)

RN 777881-25-1 CAPLUS

CN Pyridine, 3-[3-fluoro-5-[1-(2-pyridinyl)-1H-pyrazol-4-yl]phenyl]-4-methyl-(CA INDEX NAME)

RN 777881-29-5 CAPLUS

CN 1H-Pyrrolo[2,3-c]pyridine, 1-[3-chloro-5-[1-(2-pyridiny1)-1H-pyrazol-4-yl]pheny1]- (CA INDEX NAME)

RN 777881-33-1 CAPLUS

CN Pyridine, 2-[4-[3-fluoro-4-(2-pyridinyl)phenyl]-1H-pyrazol-1-yl]- (CA INDEX NAME) 10/551,709

777881-94-4 CAPLUS RN

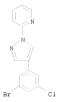
CN Pyridine, 2-(4-[1,1'-bipheny1]-3-y1-1H-pyrazol-1-y1)- (CA INDEX NAME)

777882-02-7P IT

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of diaryl pyrazole modulators of metabotropic glutamate receptor-5)

RN

777882-02-7 CAPLUS
Pyridine, 2-[4-(3-bromo-5-chlorophenyl)-1H-pyrazol-1-yl]- (CA INDEX NAME) CN



L4 ANSWER 24 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:796496 CAPLUS

DOCUMENT NUMBER: 141:290547
TITLE: Fungicidal compo

TITLE: Fungicidal compositions comprising

N-phenyl-N-[4-(4-pyridyl)-2-pyrimidin-2-yl]amine

derivatives

INVENTOR(S): Ackerman, Peter; Stierli, Daniel; Jung, Pierre Marcel Joseph; Maienfisch, Peter; Cederbaum, Fredrik Emil

Malcolm; Wenger, Jean-Frederic

PATENT ASSIGNEE(S): Syngenta Participations AG, Switz. SOURCE: Brit. UK Pat. Appl., 112 pp.

CODEN: BAXXDU

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

GI

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2399754	A	20040929	GB 2004-3967	20040223
PRIORITY APPLN. INFO.:			GB 2003-7269 A	20030328

OTHER SOURCE(S): MARPAT 141:290547

AB Compns. for protecting plants, especially fungicidal compns., comprise N-phenyl-N-[4-(4-pyridyl)-2-pyrimidin-2-yl]amine derivs. (I, Rl = halo or (un) substituted alkyl, alkoxy, alkenyloxy, alkynyloxy, thioalkyl, aryl,

Ι

etc.; R2-R9 = H, (un)substituted alkyl, aryl, etc.; R10 = H, (un) substituted alkyl, alkenyl, etc.; R11 = H, C1-4 alkyl, C3-4 alkenyl, etc.; m = 0, 1, 2, or 3; n, p = 0 or 1; q = 1 or 2) or a salt thereof, together with a suitable carrier and optionally addnl. active compds. Thus, spraying 1-wk-old wheat plants 0.02% I (in a test with 7 such compds.) resulted in >70% control of fungal infection assessed 10 days after inoculation with Puccinia graminis. 764698-85-3

RL: AGR (Agricultural use); BSU (Biological study, unclassified); BIOL

(Biological study); USES (Uses) (as fungicide for plant protection)

764698-85-3 CAPLUS RN CN

2-Pyrimidinamine, N-(3-chlorophenyl)-4-[2-(3,5-dimethyl-4-phenyl-1Hpyrazol-1-yl)-4-pyridinyl]- (CA INDEX NAME)

3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 25 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:654838 CAPLUS

DOCUMENT NUMBER: 141:325154

Discovery of Novel Heteroarvlazoles That Are TITLE:

Metabotropic Glutamate Subtype 5 Receptor Antagonists with Anxiolytic Activity

Roppe, Jeffrey; Smith, Nicholas D.; Huang, Dehua; AUTHOR(S):

Tehrani, Lida; Wang, Bowei; Anderson, Jeffrey; Brodkin, Jesse; Chung, Janice; Jiang, Xiaohui; King, Christopher; Munoz, Benito; Varney, Mark A.; Prasit,

Petpiboon; Cosford, Nicholas D. P.

CORPORATE SOURCE: Merck Research Laboratories, San Diego, CA, 92121, USA

SOURCE: Journal of Medicinal Chemistry (2004), 47(19),

4645-4648

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:325154

The highly potent, selective, and brain-penetrant metabotropic glutamate subtype 5 (mGlu5) receptor antagonists

3-(5-pyridin-2-y1-2H-tetrazo1-2-y1)benzonitrile and

3-fluoro-5-(5-pyridin-2-yl-2H-tetrazol-2-yl)benzonitrile are reported. Compound 3-(5-pyridin-2-yl-2H-tetrazol-2-yl)benzonitrile is active in the rat fear-potentiated startle (FPS) model of anxiety with ED50 = 5.4 mg/kg (po) when dosed acutely. In this model the anxiolytic effects of 3-(5-pyridin-2-v1-2H-tetrazol-2-v1)benzonitrile rapidly tolerate on repeated dosing.

546141-95-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(discovery of novel heteroarylazoles that are metabotropic glutamate subtype 5 receptor antagonists with anxiolytic activity)

546141-95-1 CAPLUS

CN Benzonitrile, 3-[1-(2-pyridinyl)-1H-pyrazol-4-yl]- (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 26 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:596910 CAPLUS DOCUMENT NUMBER: 141:410885

TITLE: Synthesis and some reactions of

4-benzoyl-5-phenyl-1-pyridin-2-yl-1H-pyrazole-3-

carboxylic acid

AUTHOR(S): Sener, Ahmet; Akbas, Esvet; Sener, M. Kasim CORPORATE SOURCE: Art and Science Faculty, Chemistry Department,

Yuezuencue Yil University, Van, 65080, Turk. SOURCE:

Turkish Journal of Chemistry (2004), 28(3), 271-277

CODEN: TJCHE3; ISSN: 1300-0527 PUBLISHER:

Scientific and Technical Research Council of Turkey

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:410885

AR The 1H-pyrazole-3-carboxylic acid (I), obtained from the furandione and 2-hydrazinopyridine, was decarboxylated to give 4-benzoyl-5-phenyl-1-pyridin-2-yl-pyrazole derivative Some ester derivs. of I were prepared by the Fischer esterification reactions of I with various alcs. Cyclocondensation reactions of I with Ph hydrazine or hydrazine hydrate led to the formation of derivs. of pyrazolo[3,4-d]pyridazine derivs.

791112-66-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reactions of 4-benzoyl-5-phenyl-1-pyridin-2-yl-1H-pyrazole-3-carboxylic acid)

791112-66-8 CAPLUS RN

CN 1H-Pyrazole-3-carboxylic acid, 4-benzoyl-5-phenyl-1-(2-pyridinyl)- (CA INDEX NAME)

IT 791112-67-9P 791112-68-0P 791112-69-1P

791112-70-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and reactions of 4-benzoy1-5-pheny1-1-pyridin-2-y1-1H-pyrazole-3-carboxylic acid)

RN 791112-67-9 CAPLUS

CN Methanone, phenyl[5-phenyl-1-(2-pyridinyl)-1H-pyrazol-4-yl]- (CA INDEX NAME)

RN 791112-68-0 CAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 4-benzoyl-5-phenyl-1-(2-pyridinyl)-, propyl ester (CA INDEX NAME)

RN 791112-69-1 CAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 4-benzoyl-5-phenyl-1-(2-pyridinyl)-, methyl ester (CA INDEX NAME)

RN 791112-70-4 CAPLUS CN

1H-Pyrazole-3-carboxylic acid, 4-benzoyl-5-phenyl-1-(2-pyridinyl)-, butyl ester (CA INDEX NAME)

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 27 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN 2004:566549 CAPLUS

ACCESSION NUMBER: DOCUMENT NUMBER:

141:123620

TITLE: Preparation of pyrazole derivatives as inhibitors of mitogen activated protein kinase-activated protein

INVENTOR(S): Hanau, Cathleen E.; Mershon, Serena Marie; Graneto, Matthew J.; Meyers, Marvin J.; Hegde, Shridhar G.;

Buchler, Ingrid P.; Wu, Kun K.; Liu, Shuang; Nacro, Kassoom

PATENT ASSIGNEE(S): Pharmacia Corporation, USA SOURCE: PCT Int. Appl., 265 pp.

CODEN: PIXXD2

Patent English

LANGUAGE: FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

DOCUMENT TYPE:

PATENT NO. KIND DATE APPLICATION NO. DATE WO 2004058176 A2 20040715 WO 2003-US40932 20031219 WO 2004058176 A3 20040916 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,

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BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2510298
                               20040715
                                           CA 2003-2510298
                                                                   20031219
                         A1
     AU 2003301226
                          A1
                                20040722
                                            Att 2003-301226
                                                                   20031219
     AU 2003301226
                          A2
                                20040722
                                           US 2003-742494
     US 20040152739
                          A1
                                20040805
                                                                   20031219
     US 20040209897
                          A1
                                20041021
                                           US 2003-742072
                                                                   20031219
     EP 1572682
                          A2
                               20050914
                                            EP 2003-814309
                                                                   20031219
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     BR 2003017525
                          Α
                               20051116
                                            BR 2003-17525
                                                                   20031219
     CN 1747949
                          Α
                                20060315
                                            CN 2003-80109626
                                                                   20031219
     JP 2006511583
                          Т
                                20060406
                                            JP 2004-563946
                                                                   20031219
     IN 2005CN01270
                               20070622
                                            IN 2005-CN1270
                          Α
                                                                   20050615
     MX 2005PA06568
                          Α
                                20050922
                                            MX 2005-PA6568
                                                                   20050617
                                            US 2007-958229
     US 20080113971
                          A1
                               20080515
                                                                   20071217
PRIORITY APPLN. INFO .:
                                            US 2002-434962P
                                                                P 20021220
                                            US 2003-742494
                                                                A1 20031219
                                            WO 2003-US40932
                                                               W 20031219
                        MARPAT 141:123620
OTHER SOURCE(S):
GΙ
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Title compds. were prepared as inhibitors of mitogen activated protein kinase-activated protein kinase-2 (MK-2). Thus, the title compound I was prepared in a multi-step synthesis and had IC50 for MK-2 inhibition of 0.0269 uM.

ΙT 723339-59-1P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrazole derivs. as inhibitors of mitogen activated protein kinase-activated protein kinase-2) 723339-59-1 CAPLUS

RN

CN 4H-Pvrazolo[1,5-a][1,4]diazepin-4-one, 5, 6, 7, 8-tetrahydro-2-[2-(4-phenyl-1H-pyrazol-1-yl)-4-pyridinyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 723339-58-0 CMF C21 H18 N6 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

SOURCE:

L4 ANSWER 28 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2003:837049 CAPLUS

DOCUMENT NUMBER: 139:337966

TITLE:

Preparation of

pyrazolylphenethylaminocarbonylbenzenesulfonamides and

related compounds as antiinflammatories and

analgesics.

INVENTOR(S): Hirano, Misato; Nakao, Kazunari; Nukui, Seiji;
Yamagishi, Tatsuya

Pfizer Pharmaceuticals Inc., Japan; Pfizer Inc.

PCT Int. Appl., 162 pp.

CODEN: PIXXD2 Patent

ANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

DOCUMENT TYPE:

PATENT ASSIGNEE(S):

PATENT NO. KIND APPLICATION NO. DATE DATE 20031023 WO 2003-IB1277 WO 2003087061 A1 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG CA 2482382 A1 20031023 CA 2003-2482382 20030402 AU 2003-216581 AU 2003216581 A.1 20031027 20030402 20050112 EP 1495005 A1 EP 2003-712488 20030402 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,

IE, SI,	LT, LV, FI	, RO, MK, 0	CY, AL, TR, BG, CZ,	EE, HU, SK
BR 2003009188	A	20050209	BR 2003-9188	20030402
JP 2005532291	T	20051027	JP 2003-584017	20030402
US 20040019045	A1	20040129	US 2003-409881	20030409
US 7001917	B2	20060221		
MX 2004PA09960	A	20041213	MX 2004-PA9960	20041011
PRIORITY APPLN. INFO.	:		US 2002-372047P	P 20020412
			WO 2003-IB1277	W 20030402
OTHER SOURCE(S):	MARPAT	139:33796	5	

R3 N NABXCONHSO2R4

AB Title compde. [I; R1 = H, alkyl, amino, mono— or dialkylamino, (substituted) aryl, heteroaryl; R2 = H, halo, alkyl, cycloalkyl, cycloalkyl, aralkyl, (substituted) aryl, heteroaryl; R3 = alkyl, haloalkyl, hydroxyalkyl, (substituted) aryl, heteroaryl; R3 = alkyl, haloalkyl, hydroxyalkyl, (substituted) aryl, heteroaryl; R3 = alkylene; X = NH, alkylimino, O, S], were prepared for treatment of prostaglandin-mediated disease such as pain, fever, and inflammation (no data). Thus, 2-(4-hydrazinophenyl)ethanol hydrochloride and benzoyl-1,1,1-trifluoroacetone were refluxed together overnight to give 56% 2-4-[5-phenyl-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]ethanol. The latter was stirred with p-toluenesulfonyl isocyanate in CH2Cl2 for 30 min. to give 73% 2-[4-[5-phenyl-3-(trifluoromethyl)-1H-pyrazol-1-yl]phenyl]ethyl

(4-methylphenyl)sulfonylcarbamate. IT 616878-30-9P 616878-31-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrazolylphenethylaminocarbonylbenzenesulfonamides and related compds. as antiinflammatories and analgesics) 616878-30-9 CAPLUS

RN 616878-30-9 CAPLUS CN Benzenesulfonamide.

Benzenesulfonamide, 4-chloro-N-[[[2-[6-(3,5-dimethyl-4-phenyl-1H-pyrazol-1-y1)-3-pyridinyl]ethyl]amino]carbonyl]-, sodium salt (1:1) (CA INDEX NAME)

Ι

N. .

RN

CN 1,3-Benzenedisulfonamide, N1-[[[2-[6-(3,5-dimethyl-4-phenyl-1H-pyrazol-1-yl)-3-pyridinyl]ethyl]amino]carbonyl]-, sodium salt (1:1) (CA INDEX NAME)

Na

IT 616879-81-3P 616879-82-4P 616879-83-5P 616879-84-6P 616879-86-8P 616879-87-9P

616879-88-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrazolylphenethylaminocarbonylbenzenesulfonamides and related compds. as antiinflammatories and analgesics)

RN 616879-81-3 CAPLUS

CN 3-Pyridinecarboxylic acid, 6-(3,5-dimethyl-4-phenyl-1H-pyrazol-1-yl)-, ethyl ester (CA INDEX NAME)

RN 616879-82-4 CAPLUS

CN 3-Pyridinemethanol, 6-(3,5-dimethyl-4-phenyl-1H-pyrazol-1-yl)- (CA INDEX NAME)

RN 616879-83-5 CAPLUS

CN 3-Pyridineacetonitrile, 6-(3,5-dimethyl-4-phenyl-1H-pyrazol-1-yl)- (CA INDEX NAME)

RN 616879-84-6 CAPLUS

CN 3-Pyridineethanamine, 6-(3,5-dimethyl-4-phenyl-1H-pyrazol-1-yl)- (CA INDEX NAME)

RN 616879-86-8 CAPLUS

CN Carbamic acid, [2-[6-(3,5-dimethyl-4-phenyl-1H-pyrazol-1-yl)-3pyridinyl]ethyl]-, phenyl ester (9CI) (CA INDEX NAME)

RN 616879-87-9 CAPLUS

CN Benzenesulfonamide, 4-chloro-N-[[[2-[6-(3,5-dimethyl-4-phenyl-1H-pyrazol-1-yl)-3-pyridinyl]ethyl]amino]carbonyl]- (CA INDEX NAME)

RN 616879-88-0 CAPLUS

CN 1,3-Benzenedisulfonamide, N1-[[[2-[6-(3,5-dimethyl-4-phenyl-1H-pyrazol-1-yl)-3-pyridinyl]ethyl]amino]carbonyl]- (CA INDEX NAME)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 29 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:491179 CAPLUS

DOCUMENT NUMBER: 139:53017

TITLE: Preparation of heteroaryl substituted pyrazole modulators of metabotropic glutamate receptor-5

INVENTOR(S): Cosford, Nicholas D. P.; Chen, Chixu; Eastman, Brian
W.; Huang, Dehua; Munoz, Benito; Prasit, Petpiboon;
Smith, Nicholas D.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA SOURCE: PCT Int. Appl., 131 pp. CODEN: PIXXD2

DOCUMENT TYPE: Pater

LANGUAGE: English FAMILY ACC. NUM. COUNT: 5

PATENT INFORMATION:

PAT	TENT	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D	ATE		
WO	2003	0518	33		A2		2003	0626		WO 2	002-	JS40:	147		20021213			
WO	2003	0518	33		A3 20031030													
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KR,	KZ,	LC,	LK,	LR,	LS,	
		LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,	PL,	
		PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	
		UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW								
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,	
		KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	
		FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	SI,	SK,	TR,	BF,	BJ,	
		CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG			
CA	2469	813			A1		2003	0626		CA 2	002-	2469	813		2	0021	213	
AU	2002	3597	14		A1	A1 20030630 AU 2002-359714												
AU	2002	3597	14		D?		2006											
EP 1458383							2004	0922		EP 2	002-	7942	67		2	0021	213	
EP	1458	383			B1		2007	1121										
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
		ΙE,	SI,	LT,			RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	SK			
	2005		34				2005	0609			003-		20		2	0021	213	
ES	2295	441								ES 2	002-	7942		2	0021	213		
	2004				A2 20040415					WO 2	003-	US97	20030331					
WO	2004	0306	37		A3		2004	0923										
	W:										BG,							
											EE,							
											KG,							
											MW,							
											SK,		ΤJ,	TM,	TN,	TR,	TT,	
											ZM,							
	RW:										TZ,							
											CH,							
											NL,							
		BF,									GW,			NE,				
	2003				A1 20040423 AU 2003-218462									0030				
US	2005	0026	963		A1		2005	0203	US 2004-497122 US 2001-341382P						20040526			
ORITY	Y APP	LN.	INFO	.:									82P	1	P 2	0011	218	
											002-			- 1				
										WO 2	002-	US40:	147	1	N 2	0021	213	

AB

WO 2002-US41720 A 20021213 WO 2002-US40237 A 20021216 WO 2002-US40486 A 20021217 WO 2003-US9717 W 20030331

OTHER SOURCE(S): MARPAT 139:53017

Pyrazole compds. substituted directly, or by a bridge, with a heteroaryl moiety containing N adjacent to the point of connection of the heteroaryl (shown as I; variables defined below; e.g. 3-[4-(pvridin-2-vl)-1H-pvrazol-1-vl]benzonitrile), are mGluR5 modulators useful in the treatment of psychiatric and mood disorders such as, for example, schizophrenia, anxiety, depression, bipolar disorder and panic, as well as in the treatment of pain, circadian rhythm disorders, and other diseases. Compds. I have mGluR5 inhibitory activity as shown by an IC50 value of <10 μM and/or an inhibition of >30% at a concentration of 3 μM in the Ca flux assay and/or inhibition of >50% at a concentration of 100 μM in the phosphatidylinositol hydrolysis assay. For I: X and Y each independently is aryl or heteroaryl wherein at least one of X and Y is a heteroaryl with N adjacent to the position of attachment to A or B resp.; A is -C0-4-alkyl, -C0-2alkyl-S0-C0-2-alkyl-, -C0-2-alkyl-S02-C0-2alkyl-, -C0-2-alkyl-C0-C0-2-alkyl-, -C0-2-alkyl-NR9C0-C0-2-alkyl-, -C0-2-alkyl-NR9S02-C0-2-alkyl- or -heteroC0-4alkyl. B is -C0-4-alkyl, -C0-2-alkyl-S0-C0-2-alkyl-, -C0-2alkyl-S02-C0-2alkyl-, -C0-2-alkyl-C0-C0-2-alkyl-, -C0-2-alkyl-NR10C0-C0-2-alkyl-, -C0-2-alkyl-NR10S02-C0-2alkyl- or -heteroC0-4alkyl; one of A1 and A2 is N, the other is CR12; R11 and R12 is each independently halogen, -C0-6alkyl, -C0-6alkoxyl, or -N(C0-4-alkyl)(C0-4-alkyl), wherein optionally R11 and R12 are combined to form a cycloalkyl, heterocycloalkyl, aryl or heteroarvl ring fused to the pyrazole moiety; any N may be an N-oxide; addnl. details including provisos are given in the claims. Although the methods of preparation are not claimed, 15 example prepns. of I and 12 example prepns. of intermediates are included; characterization data are included for an addnl. .apprx.270 examples of I.

546141-95-1P, 3-[1-(Pyridin-2-y1)-1H-pyrazol-4-y1]benzonitrile TT 546141-96-2P, 2-[4-(3-Chlorophenyl)-1H-pyrazol-1-yl]pyridine 546141-97-3P, 2-[4-(3-Methoxyphenyl)-1H-pyrazol-1-yl]pyridine 546142-41-0P, 2-[4-(2-Chlorophenyl)-1H-pyrazol-1-yl]pyridine 546142-42-1P, 2-[4-(3-Methylphenyl)-1H-pyrazol-1-yl]pyridine 546142-81-8P, 2-[4-[3-Fluoro-5-(pyridin-3-yloxy)phenyl]-1H-pyrazol-1-v1]pvridine 546142-93-2P, 2-[4-(4-Fluorophenvl)-1H-pvrazol-1-vl]pvridine 546142-94-3P, 4-[1-(Pyridin-2-y1)-1H-pyrazol-4-y1]benzonitrile 546142-95-4P, 2-[4-[3-(Trifluoromethyl)phenyl]-1H-pyrazol-1-yl]pyridine 546142-96-5P, 2-[4-[4-(Trifluoromethyl)phenyl]-1H-pyrazol-1vl]pyridine 546142-98-7P, 2-[4-(3-Fluorophenyl)-1H-pyrazol-1-yl]pyridine 546142-99-8P, 2-[4-(3,5-Dichlorophenyl)-1H-pyrazo1-1-yl]pyridine 546143-00-4P, 2-[4-(3,5-Difluorophenyl)-1H-pyrazol-1-yl]pyridine RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of heteroaryl substituted pyrazole inhibitors of metabotropic glutamate receptor-5)

RN 546141-95-1 CAPLUS

CN Benzonitrile, 3-[1-(2-pyridinyl)-1H-pyrazol-4-yl]- (CA INDEX NAME)

RN 546141-96-2 CAPLUS

CN Pyridine, 2-[4-(3-chlorophenyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)

RN 546141-97-3 CAPLUS

CN Pyridine, 2-[4-(3-methoxyphenyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)

- RN 546142-41-0 CAPLUS
- CN Pyridine, 2-[4-(2-chlorophenyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)

- RN 546142-42-1 CAPLUS
- CN Pyridine, 2-[4-(3-methylphenyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)

- RN 546142-81-8 CAPLUS
- CN Pyridine, 2-[4-[3-fluoro-5-(3-pyridinyloxy)phenyl]-1H-pyrazol-1-yl]- (CA INDEX NAME)

- RN 546142-93-2 CAPLUS
- CN Pyridine, 2-[4-(4-fluorophenyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)

10/551,709

RN 546142-94-3 CAPLUS CN Benzonitrile, 4-[1-(2-pyridiny1)-1H-pyrazo1-4-y1]- (CA INDEX NAME)

RN 546142-95-4 CAPLUS

CN Pyridine, 2-[4-[3-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]- (CA INDEX NAME)

10/551,709

- RN 546142-96-5 CAPLUS
- CN Pyridine, 2-[4-[4-(trifluoromethyl)phenyl]-1H-pyrazol-1-yl]- (CA INDEX NAME)

- RN 546142-98-7 CAPLUS
- CN Pyridine, 2-[4-(3-fluorophenyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)

- RN 546142-99-8 CAPLUS
- CN Pyridine, 2-[4-(3,5-dichlorophenyl)-1H-pyrazol-1-yl]- (CA INDEX NAME)

RN 546143-00-4 CAPLUS

Pyridine, 2-[4-(3,5-difluorophenyl)-1H-pyrazol-1-yl]- (CA INDEX NAME) CN



L4 ANSWER 30 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:112122 CAPLUS

DOCUMENT NUMBER: 139:239629

TITLE:

CoMFA and CoMSIA studies of angiotensin (AT1) receptor antagonists

AUTHOR(S):

Datar, Prasanna; Desai, Prashant; Coutinho, Evans; Iyer, Krishna

CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Bombay College

of Pharmacy, Mumbai, 400 098, India

Journal of Molecular Modeling (2002), 8(10), 290-301 SOURCE:

CODEN: JMMOFK; ISSN: 0948-5023 URL: http://link.springer.de/link/service/journals/008

94/contents/02/00097/paper/s00894-002-0097-6.pdf

PUBLISHER: Springer-Verlag

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

Two 3D-QSAR methods CoMFA and CoMSIA were applied to a set of 38 angiotensin receptor (AT1) antagonists. The conformation and alignment of mols, were obtained by a novel method consensus dynamics. The representation of biol. activity, partial charge formalism, absolute orientation of the mols. in the grid, and grid spacing were also studied for their effect on the CoMFA models. The models were thoroughly validated through trials using scrambled activities and bootstrapping. The best CoMFA model had across-validated correlation coefficient (g2) of 0.632, which improved with "region focusing" to 0.680. This model had a "predictive" r2 of 0.436 on a test series that was unique and with little representation in the training set. Although the "predictive" r2 of the best CoMSIA model, which included steric, electrostatic, and hydrogen bond acceptor fields was higher than that of the best CoMFA model, the other statistical parameters like q2, r2, F value, and s were unsatisfactory. The contour maps generated using the best CoMFA model were used to identify the structural features important for biol. activity in these

compds. 152713-36-5

RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(CoMFA and CoMSIA studies of angiotensin (AT1) receptor antagonists) 152713-36-5 CAPLUS RN

CN 1H-Pyrazole-5-carboxylic acid, 3-butyl-1-(2-pyridinyl)-4-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, ethyl ester (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 31 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

54

ACCESSION NUMBER: 2002:293632 CAPLUS

DOCUMENT NUMBER: 136:325538

TITLE: Preparation of pyrazoles for the treatment of viral

diseases

INVENTOR(S): Dymock, Brian William; Jones, Philip Stephen; Merrett,
John Herbert; Parratt, Martin John

PATENT ASSIGNEE(S): F. Hoffmann-La Roche Ag, Switz.

SOURCE: PCT Int. Appl., 108 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	ENT I										ICAT					DATE	
WO	2002	0309	07		A1 20020418			WO 2001-EP11474					20011004				
	W:	CO, GM,	CR, HR,	CU, HU,	CZ, ID,	DE, IL,	AU, DK, IN,	DM, IS,	DZ, JP,	EC, KE,	EE, KG,	ES, KP,	FI, KR,	GB, KZ,	GD, LC,	GE, LK,	GH, LR,
		PT, UZ,	RO, VN,	RU, YU,	SD, ZA,	SE, ZW	MD, SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,
	RW:	DE,	DK,	ES,	FI,	FR,	MZ, GB, GA,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	
				A1 20030123				US 2001-956656							920		
US	6699	887			B2		2004	0302									
CA	2423	515			A1		2002	0418		CA 2	001-	2423.	515		2	0011	004
ΑU	2002	0216	51		A 20020422			AU 2002-21651					20011004				
									BR 2001-14483					20011004			
EΡ	1326	843			A1		2003	0716		EP 2	001-	9866	80		2	0011	004
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
							RO,										
	2003																
JP	2004 4015	548			B2		2007	1128								0011	
	5247															0011	004
CN	1680	333			A		2005	1012		CN 2	005-	1000	8832		2	0011	004

RU	2270832	C2	20060227	RU	2003-112610		20011004
AU	2002221651	B2	20061019	AU	2002-221651		20011004
ZA	2003002519	A	20040630	zA	2003-2519		20030331
IN	2003CN00492	A	20050415	IN	2003-CN492		20030407
MX	2003PA03070	A	20030714	MX	2003-PA3070		20030408
NO	2003001615	A	20030523	NO	2003-1615		20030409
US	20040192752	A1	20040930	US	2004-766712		20040127
US	7183296	B2	20070227				
HK	1061021	A1	20050527	HK	2004-103975		20040603
PRIORITY	APPLN. INFO.:			GB	2000-24795	A	20001010
				US	2001-956656	A3	20010920
				CN	2001-817171	A3	20011004
				WO	2001-EP11474	W	20011004

OTHER SOURCE(S): MARPAT 136:325538

GI

AB The title compds. [I; Rl = alkyl, cycloalkyl, aryl, etc.; R2 = aryl, (un) substituted Ph; R3 = alkyl, alkoxyalkyl; A = CH2(arylalkylamino), CH2(arylalkoxyl, etc.; X = S, O] that are inhibitors of the human immunodeficiency virus reverse transcriptase enzyme which is involved in viral replication, were prepared E.g., a 3-step synthesis of pyrazole I [Rl = Ph; R2 = 3,5-Cl2C6H3; X = S; R3 = Me; A = CH2Ph] which showed IC50 of 2060 nM against HIV-1 reverse transcriptase, was given.

412326-26-2P RI: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrazoles as inhibitors of the HIV reverse transcriptase)

RN 412326-26-2 CAPLUS

CN Pyridine, 2-[5-[(3,5-dichlorophenyl)thio]-3-methyl-4-(phenylmethyl)-1Hpyrazol-1-yl]- (CA INDEX NAME)

REFERENCE COUNT:

1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 32 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2000:813020 CAPLUS DOCUMENT NUMBER: 134:128105

TITLE: Miniature single-particle immunoassay for

prostate-specific antigen in serum using recombinant

Fab fragments

AUTHOR(S): Harma, Harri; Tarkkinen, Piia; Soukka, Tero; Lovgren,

Timo

CORPORATE SOURCE: Department of Biotechnology, University of Turku,

Turku, FIN-20520, Finland

SOURCE: Clinical Chemistry (Washington, D. C.) (2000), 46(11),

1755-1761

CODEN: CLCHAU; ISSN: 0009-9147

PUBLISHER: American Association for Clinical Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

Background: Quant., miniaturized nucleic acid assays and immunoassays can be developed with single microparticles, microfluorometric detection, and intrinsically fluorescent lanthanide chelates in a multiple assay format to decrease reagent consumption, cost, and assay time. We used recombinant Fab fragments to capture and detect free and total prostate-specific antigen (PSA) from serum in a submicroliter volume single-particle immunoassay. Methods: Genetically engineered thiol-Fab or thiolated monoclonal antibodies (mAbs) were covalently attached onto uniformly sized 60-µm maleimide-activated microparticles. Free and total PSA were detected with europium- or terbium-labeled Fab fragments on a single microparticle using a microfluorometer in a time-resolved mode. Results: The detection limit of the free- and total-PSA assays (mean + 3 SD of zero calibrator) was 0.35 $\mu g/L$, with a total volume of 330 nL per particle. An excellent correlation was found in microparticle and microtiter-well assays for 21 serum samples: slopes for free and total PSA were 1.06 ± 0.03 and 1.03 ± 0.02 , resp. (Sy/x = 0.084) and 0.057μg/L), with intercepts of 0.013±0.018 and 0.013±0.017 μg/L (R >0.99). Furthermore, the particle-immobilized Fab fragment had a PSA binding capacity 1.5-fold higher than the intact mAb capacity on a single microparticle. Capacity, kinetics, and sensitivity of the Fab fragment and intact mAb assays in the microparticle and microtiter well formats are discussed. Conclusions: With site-specific (cysteine tail) covalent attachment of Fab fragments on a microparticle, subattomole amts. of PSA can be detected quant.

321883-66-3D, europium and terbium complexes

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (fluorescent label for mAb; miniature single-particle immunoassay for prostate-specific antigen in serum using recombinant Fab fragments)

RN 321883-66-3 CAPLUS CN Glycine, N.N'-[[4-]]

Glycine, N,N'-[[4-[2-(4-isothiocyanatophenyl)ethyl]-1H-pyrazole-1,3-diyl]bis(6,2-pyridinediylmethylene)]bis[N-(carboxymethyl)- (9CI) (CA INDEX NAME)

24 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 33 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:124064 CAPLUS DOCUMENT NUMBER: 132:175822

TITLE: 3,4-substituted pyrazoles for the treatment of

inflammation

INVENTOR(S): Lee, Len F.; Penning, Thomas D.; Kramer, Steven W.; Talley, John J.

THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS

PATENT ASSIGNEE(S): G.D. Searle and Co., USA

SOURCE: U.S., 42 pp., Cont.-in-part of U.S. 5,486,534

CODEN: USXXAM DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

REFERENCE COUNT:

PAT	TENT	NO.			KIN	D	DATE			APPL	ICAT	ION:	NO.		D.	ATE	
US	6028	072			A 20000222				US 1997-776090					19970609			
US	5486	534			A 19960123					US 1994-278297					19940721		
WO	9603	385			A1		1996	0208		WO 1	995-	US87	88		1	9950	720
	₩:	AM,	AT,	AU,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CZ,	DE,	DK,	EE,	ES,	FI,
		GB,	GE,	HU,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LK,	LR,	LT,	LU,	LV,	MD,
		MG,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	TJ,
		TM,	TT														
	RW:	KE,	MW,	SD,	SZ,	UG,	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IE,	IT,
		LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	ML,	MR,	NE,
		SN,	TD,	TG													
PRIORITY	Y APP	LN.	INFO	. :						US 1	994-	2782	97		A2 1	9940	721
										WO 1	995-	us87	88		W 1	9950	720

OTHER SOURCE(S): MARPAT 132:175822

A class of pyrazolyl compds. (Markush included) is described for use in treating inflammation and inflammation-related disorders. Compound preparation is included.

259172-55-9 259173-36-9

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(pyrazole derivative preparation for treatment of inflammation and inflammation-related disorders)

RM 259172-55-9 CAPLUS CN Pyridine, 2-[2-[4-[4-(methylsulfonyl)phenyl]-3-(4-pyridinyl)-5-(trifluoromethyl)-1H-pyrazol-1-yl]ethyl]- (CA INDEX NAME)

RN 259173-36-9 CAPLUS

CN Benzenesulfonamide, 4-[3-(4-pyridinyl)-1-[2-(2-pyridinyl)ethyl]-5-(trifluoromethyl)-1H-pyrazol-4-vl]- (CA INDEX NAME)

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 34 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:117030 CAPLUS

DOCUMENT NUMBER: 2000:117030 CAPLOS

TITLE: Preparation of estrogen receptor modulating pyrazoles
INVENTOR(S): Huebner, Verena D.; Lin, Xiaodong; James, Ian; Chen,
Liya; Desai, Manoj; Krywult, Beata; Sindh, Rajinder;

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS

Wang, Liang
PATENT ASSIGNEE(S): Chiron Corp., USA

SOURCE: PCT Int. Appl., 124 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

REFERENCE COUNT:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000007996	A2	19990806	WO 1999-US17799	19990806

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WO 2000007996 A3 20000831
        W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ,
             DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,
            JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK,
            MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ,
             TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,
             ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG,
             CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     AU 9954677
                         A
                              20000228 AU 1999-54677
                                                                   19990806
     EP 1102753
                         A2
                               20010530
                                           EP 1999-940917
                                                                  19990806
     EP 1102753
                         B1
                              20070228
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, CY
     US 6291505
                         В1
                              20010918
                                           US 1999-369747
                                                                   19990806
                                           JP 2000-563630
     JP 2002522422
                         T
                               20020723
                                                                   19990806
     AT 355279
                         T
                               20060315
                                            AT 1999-940917
                                                                   19990806
     ES 2281186
                        Т3
                               20070916
                                           ES 1999-940917
                                                                   19990806
     US 20020111374
                        A1
                               20020815
                                           US 2001-954039
                                                                   20010918
     US 20040034081
                         A9
                               20040219
                               20040427
     US 6727273
                         B2
     US 20040077701
                              20040422
                         A1
                                           US 2003-461914
                                                                   20030612
                         E1 20070626
     US 39708
                                            US 2004-757347
                                                                   20040113
                                                              P 19980807
P 19980807
PRIORITY APPLN. INFO.:
                                            US 1998-95772P
                                            US 1998-95773P
                                            US 1999-369747 A3 19990806
WO 1999-US17799 W 19990806
US 2001-954039 A1 20010918
OTHER SOURCE(S):
                       MARPAT 132:166234
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- AB The title compds. [I and II; Rl, R3 = alkyl, aryl, heteroaryl, etc.; R2 = H, halo, CN, etc.; R4 = H, CO2H, CHO, etc.] which have been found to have unexpected and surprising activity in modulating estrogen receptor activity, and therefore are useful for treating or preventing estrogen receptor—mediated disorders such as osteoporosis, breast and endometrial cancers, atherosclerosis, and Alzheimer's disease, were prepared E.g., a multi-step synthesis of II [R1 = Ph2CH; R2 = Et, R3 = 4-HOC6H4; R4 = Me], starting with 4'-methoxybutyrylphenone and 2,2-diphenylacetyl chloride, was given (no data for intermediates). Biol. data for compds. I and II were presented.
- IT 258845-91-9P 258846-07-0P 258847-06-2P 258847-10-8P 258847-11-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

- (preparation of estrogen receptor modulating pyrazoles)
- RN 258845-91-9 CAPLUS
- CN Phenol, 4,4',4''-[1-[5-chloro-3-(trifluoromethyl)-2-pyridinyl]-1H-pyrazole-

3,4,5-triy1]tris- (9CI) (CA INDEX NAME)

RN

258846-07-0 CAPLUS Phenol, 4,4',4''-[1-(2-pyridinyl)-1H-pyrazole-3,4,5-triyl]tris- (9CI) (CA CN INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 258847-06-2 CAPLUS

CN Phenol, 4,4'-[1-[6-methyl-4-(trifluoromethyl)-2-pyridinyl]-4-phenyl-1Hpyrazole-3,5-diyl]bis- (9CI) (CA INDEX NAME)

RN 258847-10-8 CAPLUS

CN Phenol, 4,4'-[1-[5-chloro-3-(trifluoromethyl)-2-pyridinyl]-4-phenyl-1H-pyrazole-3,5-diyl]bis-(9CI) (CA INDEX NAME)

RN 258847-11-9 CAPLUS

CN Phenol, 4,4'-[1-[3-chloro-5-(trifluoromethy1)-2-pyridiny1]-4-phenyl-1H-pyrazole-3,5-diyl]bis-(9CI) (CA INDEX NAME)

L4 ANSWER 35 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN 1999:819049 CAPLUS

ACCESSION NUMBER:

DOCUMENT NUMBER: 132:64173

TITLE: Preparation of labeling reactants for fluorescent

labeling of biospecific binding reactants Takalo, Harri; Hovinen, Jari; Mukkala, Veli-matti;

INVENTOR(S): Liitti, Pivi; Mikola, Heikki

PATENT ASSIGNEE(S): Wallac Oy, Finland

SOURCE: Eur. Pat. Appl., 26 pp. CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

GI

PATENT NO.	KIND DATE	APPLICATION NO.	DATE		
EP 967205	A1 19991229	EP 1999-660100	19990603		
EP 967205	B1 20030917				
R: AT, BE, CH,	DE, DK, ES, FR, GB,	GR, IT, LI, LU, NL,	SE, MC, PT,		
IE, SI, LT,	LV, FI, RO				
US 6080839	A 20000627	US 1998-104219	19980625		
PRIORITY APPLN. INFO.:		US 1998-104219	A 19980625		
OTHER SOURCE(S):	CASREACT 132:64173:	: MARPAT 132:64173			

AR Novel pyridinediylbis(methylenenitrilo)tetrakisacetic acid labeling reactants, suitable for fluorescent labeling of biospecific binding reactants in solid-phase synthesis, were prepared. The novel labeling reactants (I) [wherein A = a bivalent aromatic structure capable of absorbing light or energy and transferring the excitation energy to a lanthanide ion after the product made by solid-phase synthesis has been released from the used solid support, deprotected, and converted to a lanthanide chelate; R = -Z(G1-NH-X)G2-E; X = a transient protecting group, e.g. 2-(4-nitrophenylsulfonyl)ethoxycarbonyl, trityl, 4-methoxytrityl, 4,4'-dimethoxytrityl, BOC, Fmoc; E = a carboxylic acid, its salt, active ester (e.g. N-hydroxysuccinimido, nitrophenol, 2,4-dinitrophenol, or pentafluorophenol), or halide; Z = the bridge point; G = a bridge between A and Z; G1 = a bridge between NH and Z; G2 = a bridge between E and Z; R1 = CO2R2; R2 = alkyl or (un)substituted Ph or benzyl] are particularly useful in the labeling of small mols. Thus, II was prepared in a 4-step sequence involving (1) desilylation of Me (4-trimethylsilylethynylphenoxy)acetate (83%), (2) addition to tetra(tert-Bu) 2,2',2'',2'''-[(4-bromopyridine-2,6diyl)bis(methylenenitrilo)]tetrakis(acetate) (75%), (3) deesterification of the phenoxyacetate with KOH (67%), and (4) amidation with α -Fmoc-lysine.HCl (56%). II was used for labeling of an estradiol derivative, incorporating four Eu(III) chelates, on a solid support (no data). 253137-97-2P 253137-98-3P 253137-99-4P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of

pyridinediylbis(methylenenitrilo)tetrakisacetic acid labeling reactants for fluorescent labeling of biospecific binding reactants in solid phase synthesis)

RN 253137-97-2 CAPLUS

CN

Glycine, N,N'-[[4-[[4-(2-methoxy-2-oxoethoxy)phenyl]ethynyl]-IH-pyrazole-1,3-diyl]bis(6,2-pyridinediylmethylene)]bis[N-[2-(1,1-dimethylethoxy)-2oxoethyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

RN 253137-98-3 CAPLUS

CN Glycine, N,N'-[[4-[2-(4-(2-methoxy-2-oxoethoxy)phenyl]ethyl]-IH-pyrazole-1,3-diyl]bis(6,2-pyridinediylmethylene)]bis[N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-, bis(1,1-dimethylethyl) seter (9CI) (CA INDEX NAME)

RN 253137-99-4 CAPLUS

CN Glycine, N,N'-[[4-[2-[4-(carboxymethoxy)phenyl]ethyl]-1H-pyrazole-1,3diyl]bis(6,2-pyridinediylmethylene)]bis[N-[2-(1,1-dimethylethoxy)-2oxoethyl]-, 1,1'-bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

- IT 253137-93-8P
 - RL: SPN (Synthetic preparation); PREP (Preparation) (target compound; preparation of

pyridinediylbis(methylenenitrilo)tetrakisacetic acid labeling reactants for fluorescent labeling of biospecific binding reactants in solid phase synthesis)

- RN 253137-93-8 CAPLUS
- CN D-Lysine, N6-[[4-[2-11,3-bis[6-[[bis[2-(1,1-dimethylethoxy)-2-oxoethyl]amino]methyl-2-pyridinyl]-1-pyrazol-4-yl]ethyl]phenoxy]acetyl]-N2-[(9H-fluoren-9-ylmethoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS

REFERENCE COUNT:

3 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 36 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1999:296167 CAPLUS

DOCUMENT NUMBER: 131:44929

TITLE: Study on ferrocenes, part 6. 1,3-Dipolar cycloadditions of heterocyclic hydrazones of

formvlferrocene

AUTHOR(S): Abran, A.; Csampai, A.; Bocskei, Zs.; Sohar, P. CORPORATE SOURCE: General and Inorganic Department of Chemistry, Eotvos

Lorand University, Budapest, H-1518/112, Hung. Tetrahedron (1999), 55(17), 5441-5448 SOURCE:

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English CASREACT 131:44929

OTHER SOURCE(S): GΙ

1,3-Dipolar cycloaddn. reactions of ferrocenylmethyllidenehydrazones containing different heterocycles (la-c) with some dipolarophiles resulted in new cycloadducts and condensed triazoles. For example, the reaction of I with (E)-PhCH:CHNO2 in acetonitrile over mol. sieves under argon yielded II in 87%. The reactivity of the substrates was dependent on the heterocyclic moiety. The structure of the products was determined by IR. 1Hand 13C-NMR (1-dimensional and 2D) measurements were supported by single

crystal x-ray anal.

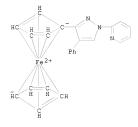
226698-83-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation via 1,3-dipolar cycloaddn. of ferrocenylmethyllidenehydrazones with various dipolarophiles)

226698-83-5 CAPLUS

Ferrocene, [4-phenvl-1-(2-pvridinvl)-1H-pvrazol-3-vl]- (9CI) (CA INDEX NAME)



THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 18 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 37 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN L4

ACCESSION NUMBER: 1998:424244 CAPLUS DOCUMENT NUMBER: 129:95503

ORIGINAL REFERENCE NO.: 129:19703a,19706a

TITLE: Preparation of pyrazoline compounds and use as plant

disease control agent

INVENTOR(S): Taki, Toshiaki; Sato, Junichi; Kimura, Norio

PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan; Taki, Toshiaki;

Sato, Junichi; Kimura, Norio

SOURCE: PCT Int. Appl., 81 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

LANGUAGE:

PA:	TENT :	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D	ATE	
WO	9827	084			A1		1998	0625		WO 1	997-	JP46	27		1	9971	216
	W:	AL,	AM,	ΑT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	DE,
		DK,	EE,	ES,	FΙ,	GB,	GE,	GW,	HU,	ID,	IL,	IS,	JP,	KE,	KG,	KR,	KZ,
		LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,
		PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	UA,	UG,	US,
		UZ,	VN,	YU,	ZW,	AM,	AZ,	BY,	KG,	KZ,	MD,	RU,	ΤJ,	TM			
	RW:	GH,	GM,	KE,	LS,	MW,	SD,	SZ,	UG,	ZW,	ΑT,	BE,	CH,	DE,	DK,	ES,	FΙ,
		FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,
		GA,	GN,	ML,	MR,	NE,	SN,	TD,	TG								
AU	9854	129			A		1998	0715		AU 1	998-	5412	9		1	9971:	216
EP	9672	12			A1		1999	1229		EP 1	997-	9479	54		1:	9971:	216

R: DE, FR, GB PRIORITY APPLN. INFO.:

MARPAT 129:95503

A 19961216 W 19971216

JP 1996-335729

WO 1997-JP4627

OTHER SOURCE(S):

AB Pyrazoline compds. represented by general formula (I; wherein R1 represents optionally substituted phenyl; R2 represents an optionally substituted hydrocarbon group; R3 represents an optionally substituted aromatic heterocyclyl; R4 and R5 are the same or different and each represents hydrogen, acyl, an optionally substituted primary or secondary alkyl; or R4 and R5 are bonded to each other to form an optionally substituted alkylene or :CR6R7; wherein R6 represents an optionally substituted hydrocarbon group, alkoxy, or mono- or dialkylamino; R7 represents H or alkvl) are prepared The compds, are used as the active ingredient of a plant disease control agent. They are useful as fungicides, in particular against mildew. Thus, 1-methylpropyl iodide was added to a mixture of 5-amino-4-(3-chlorophenyl)-1-(pyrimidin-2-yl)pyrazolin-3-one, K2CO3, and EtOH and stirred at room temperature for 72 h to give the title

compound (II), which at 2.5 mg per pot controlled ≥90% Ervsiphe graminis f.sp. tritici for wheat seedlings.

209520-93-4P 209520-95-6P 209520-96-7P 209520-97-8P 209520-98-9P 209520-99-0P

209521-00-6P 209521-01-7P 209521-02-8P 209521-03-9P 209521-04-0P 209521-05-1P

209521-06-2P 209521-08-4P 209521-09-5P

209521-10-8P 209521-11-9P 209521-12-0P

209521-13-1P 209521-14-2P 209521-15-3P

209521-16-4P 209521-17-5P 209521-18-6P

209521-21-1P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent) (preparation of pyrazoline compds. as plant disease control agents)

209520-93-4 CAPLUS RN

CN 3H-Pyrazol-3-one, 5-amino-4-(3-chlorophenyl)-1,2-dihydro-1-(2-pyridinyl)- 10/551,709

(CA INDEX NAME)

209520-95-6 CAPLUS RN CN

3H-Pyrazol-3-one, 5-amino-4-(2-chloro-6-fluorophenyl)-1,2-dihydro-1-(2-pyridinyl)- (CA INDEX NAME)

209520-96-7 CAPLUS

3H-Pyrazol-3-one, 5-amino-4-(2-chlorophenyl)-1,2-dihydro-1-(2-pyridinyl)-CN (CA INDEX NAME)

- RN 209520-97-8 CAPLUS
- CN 3H-Pyrazol-3-one, 5-amino-1,2-dihydro-4-(3-methylphenyl)-1-(2-pyridinyl)-(CA INDEX NAME)

- RN 209520-98-9 CAPLUS
- CN 3H-Pyrazol-3-one, 5-amino-1,2-dihydro-4-phenyl-1-(2-pyridinyl)- (CA INDEX NAME)

- RN 209520-99-0 CAPLUS

- RN 209521-00-6 CAPLUS
- CN 3H-Pyrazol-3-one, 5-amino-1,2-dihydro-4-(2-methylphenyl)-1-(2-pyridinyl)-(CA INDEX NAME)

10/551,709

RN 209521-01-7 CAPLUS

CN 3H-Pyrazol-3-one, 5-amino-4-(2,6-dichlorophenyl)-1,2-dihydro-1-[3-(trifluoromethyl)-2-pyridinyl]- (CA INDEX NAME)

RN 209521-02-8 CAPLUS

RN 209521-03-9 CAPLUS

CN 3H-Pyrazol-3-one, 5-amino-4-(3-chlorophenyl)-1, 2-dihydro-1-[3-(trifluoromethyl)-2-pyridinyl]- (CA INDEX NAME)

RN 209521-04-0 CAPLUS

CN 3H-Pyrazol-3-one, 5-amino-4-(2,6-dichlorophenyl)-1,2-dihydro-1-(2-pyridinyl)- (CA INDEX NAME)

RN 209521-05-1 CAPLUS

CN 3H-Pyrazol-3-one, 5-amino-1,2-dihydro-4-(4-methylphenyl)-1-(2-pyridinyl)-(CA INDEX NAME)

- RN 209521-06-2 CAPLUS
- CN 3H-Pyrazol-3-one, 5-amino-1-(5-chloro-2-pyridinyl)-4-(2,6-dichlorophenyl)-1,2-dihydro- (CA INDEX NAME)

- RN 209521-08-4 CAPLUS
- CN 3H-Pyrazol-3-one, 5-amino-4-(3-bromophenyl)-1,2-dihydro-1-(2-pyridinyl)-(CA INDEX NAME)

- RN 209521-09-5 CAPLUS
- CN 3H-Pyrazol-3-one, 5-amino-1,2-dihydro-1-(2-pyridiny1)-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

10/551,709

RN 209521-10-8 CAPLUS
CN 3H-Pyrazol-3-one, 5-amino-4-(3,4-difluorophenyl)-1,2-dihydro-1-(2-pyridinyl)- (CA INDEX NAME)

RN 209521-11-9 CAPLUS

CN 3H-Pyrazol-3-one, 5-amino-4-(3,4-dimethoxyphenyl)-1,2-dihydro-1-(2-pyridinyl)- (CA INDEX NAME)

- RN 209521-12-0 CAPLUS
- CN 3H-Pyrazol-3-one, 5-amino-4-(3,5-dichlorophenyl)-1,2-dihydro-1-(2-pyridinyl)- (CA INDEX NAME)

- RN 209521-13-1 CAPLUS
- CN 3H-Pyrazol-3-one, 5-amino-1-[4,5-bis(trifluoromethyl)-2-pyridinyl]-4-(3-chlorophenyl)-1,2-dihydro- (CA INDEX NAME)

- RN 209521-14-2 CAPLUS
- CN 3H-Pyrazol-3-one, 5-amino-1,2-dihydro-4-(4-methoxyphenyl)-1-(2-pyridinyl)- (CA INDEX NAME)

CN 3H-Pyrazol-3-one, 5-amino-4-(3-chlorophenyl)-1-(5-chloro-2-pyridinyl)-1,2-dihydro- (CA INDEX NAME)

- RN 209521-16-4 CAPLUS
- CN 3H-Pyrazol-3-one, 5-amino-1-(5-bromo-2-pyridinyl)-4-(3-chlorophenyl)-1,2dihydro- (CA INDEX NAME)

- RN 209521-17-5 CAPLUS
- CN 3H-Pyrazol-3-one, 5-amino-4-(3-chlorophenyl)-1-(3-chloro-2-pyridinyl)-1,2-dihydro- (CA INDEX NAME)

- RN 209521-18-6 CAPLUS
- CN 3H-Pyrazol-3-one, 5-amino-4-(3-chlorophenyl)-1-(6-chloro-2-pyridinyl)-1,2-dihydro- (CA INDEX NAME)

RN 209521-21-1 CAPLUS

CN 3H-Pyrazol-3-one, 5-amino-4-(3-chlorophenyl)-1,2-dihydro-1-(5-nitro-2pyridinyl) - (CA INDEX NAME)

REFERENCE COUNT:

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

30 L4 ANSWER 38 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1997:374715 CAPLUS

DOCUMENT NUMBER: 126:350804

ORIGINAL REFERENCE NO.: 126:68079a,68082a TITLE:

Biospecific binding reactants labeled with luminescent lanthanide chelates and their use INVENTOR(S):

Rodriguez-Ubis, Juan Carlos; Takalo, Harri; Mukkala,

THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS

Veli-matti

Wallac Oy, Finland; Rodriguez-Ubis, Juan Carlos PATENT ASSIGNEE(S):

SOURCE: Eur. Pat. Appl., 33 pp. CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 770610	A1	19970502	EP 1996-660056	19960909
EP 770610	B1	20050706		
R: DE, FR, GB				
US 5859215	A	19990112	US 1995-548174	19951025

GI

PRIORITY APPLN. INFO.: OTHER SOURCE(S):

MARPAT 126:350804

US 1995-548174 A 19951025

- AB This invention relates to a detectable mol. comprising a biospecific binding reactant attached to a luminescent lanthanide chelate comprising a lanthanide ion and a chelating ligand (-O2CCH2)2NCH2-[A](-G1)-CH2N(CHG2CO2-)(CH2CO2-) wherein -A- is a bivalent aromatic structure selected from pyridine-pyrazole compds. I, II, etc. and groups G1 or G2 are H, C1, Br, I, CN, Ph, alkyl, alkoxy, etc., one of which is used for coupling the chelate to a biospecific binding reactant. The lanthanide ion is Eu(III), Tb(III), Dy(III) or Sm(III). The biospecific binding reactant may be selected from a group consisting of an antibody, antigen, receptor ligand, a specific binding protein, and a DNA or RNA probe.
- 189805-29-6P 189805-30-9P 189805-36-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of luminescent lanthanide pyrazolediylbispyridinediyl and pyridinediylbispyrazolediyl bismethylenenitrilotetrakisacetato chelates for biospecific binding assays)

189805-29-6 CAPLUS RN

CN Glycine, N,N'-[[4-[(4-aminophenyl)ethynyl]-1H-pyrazole-1,3-diyl]bis(6,2pyridinediylmethylene)]bis[N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \bullet \\ \bullet \\ t-BuO-C-CH_2-N-CH_2 \\ \hline \\ N \\ \hline \end{array}$$

RN 189805-30-9 CAPLUS

Glycine, N,N'-[[4-[2-(4-aminophenyl)ethyl]-lH-pyrazole-1,3-diyl]bis(6,2pyridinediylmethylene)]bis[N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-, 1,1'-bis(1,1-dimethylethyl) ester (CA INDEX NAME)

RN 189805-36-5 CAPLUS

CN Glycine, N,N'-[[4-[2-(4-aminophenyl)ethyl]-1H-pyrazole-1,3-diyl]bis(6,2-pyridinediylmethylene)]bis[N-(carboxymethyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 39 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:965587 CAPLUS DOCUMENT NUMBER: 124:175925

ORIGINAL REFERENCE NO.: 124:32623a,32626a

ORIGINAL REFERENCE NO.: 124:32623a,32626a

TITLE: Synthesis, structure and properties of pyrazole type

tetrakis compounds
AUTHOR(S): Reiner, Knut; Richter, Rainer; Hauptmann, Siegfried;

Becher, Jan; Hennig, Lothar

CORPORATE SOURCE: Inst. Org. Chem., Univ. Leipzig, Leipzig, D-04103,

SOURCE: Tetrahedron (1995), 51(48), 13291-300 CODEN: TETRAB: ISSN: 0040-4020

PUBLISHER: Elsevier DOCUMENT TYPE: Journal LANGUAGE: English

GΙ

AB A series of pyrazole-type tetrakis compds. I (Rl = Ph, 2-pyridyl, 2-benzothiazolyl, R2 = Me, ACNH; Z = m-C6H4, p-C6H4, 2, 6-pyridinediyl, 1,10-phenanthrolidinediyl) has been synthesized by reaction of aromatic or heterocyclic dialdehydes and pyrazolone derivs. Structure and tautomerism of the products were investigated by spectroscopic methods and x-ray anal. Several tetrakis compds. form inclusion complexes with solvents like alcs., ethers, and ketones in a definite ratio via hydrogen bonds.

IT 173598-23-7P 173598-24-8P RL: SPN (Synthetic preparation); PREP (Preparation)

Ι

(preparation and inclusion reaction of tetrakis pyrazoles)
RN 173598-23-7 CAPLUS

CN 3H-Pyrazol-3-one, 4,4'-[1,3-phenylenebis[[5-hydroxy-3-methyl-1-(2-pyridinyl)-1H-pyrazol-4-yl]methylene]]bis[1,2-dihydro-5-methyl-2-(2-pyridinyl)-(9CI) (CA INDEX NAME)

- RN 173598-24-8 CAPLUS
- CN 3H-Pyrazol-3-one, 4,4'-[1,4-phenylenebis[[5-hydroxy-3-methyl-1-(2-pyridinyl)-1H-pyrazol-4-yl]methylene]]bis[1,2-dihydro-5-methyl-2-(2-pyridinyl)-(9CI) (CA INDEX NAME)

PAGE 2-A



L4 ANSWER 40 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1994:147120 CAPLUS

DOCUMENT NUMBER: 120:147120

ORIGINAL REFERENCE NO.: 120:25705a,25708a
TITLE: Pyrazolone derivatives as inhibitors of the acidic

Corrosion of steel
AUTHOR(S): Shein, A. B.; Pavlov, P. T.; Aitov, R. G.; Lesnov, A.

CORPORATE SOURCE: Perm. Gos. Univ., Perm, Russia

SOURCE: Zashchita Metallov (1993), 29(6), 940-2 CODEN: ZAMEA9; ISSN: 0044-1856

DOCUMENT TYPE: Journal

LANGUAGE: Russian

B The pyrazolone derivs. were very effective corrosion inhibitors in hydrochloric acid solns. They can be easily synthesized, are stable and

hydrochloric acid solns. They can be easily synthesized, are stable characterized by low toxicity.

IT 153231-88-0

RL: PRP (Properties)

(corrosion inhibitor, for steel, in acidic solns.)

RN 153231-88-0 CAPLUS

CN 1H-Pyrazol-5-ol, 4,4'-(phenylmethylene)bis[3-methyl-1-(2-pyridinyl)- (CA

INDEX NAME)

L4 ANSWER 41 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:134381 CAPLUS DOCUMENT NUMBER: 120:134381

ORIGINAL REFERENCE NO.: 120:23667a,23670a

TITLE: Nonpeptide angiotensin II antagonists derived from

1H-pyrazole-5-carboxylates and 4-aryl-1H-imidazole-5-carboxylates

AUTHOR(S): Ashton, Wallace T.; Hutchins, Steven M.; Greenlee,
William J.; Doss, George A.; Chang, Raymond S. L.;
Lotti, Victor J.; Faust, Kristie A.; Chen, Tsing Bau;

Zingaro, Gloria J.; et al.
CORPORATE SOURCE: Merck Res. Lab., Rahway, NJ, 07065.

CORPORATE SOURCE: Merck Res. Lab., Rahway, NJ, 07065, USA SOURCE: Journal of Medicinal Chemistry (1993), 36(23),

3595-605

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal LANGUAGE: English

AB Two series of potential angiotensin II antagonists derived from carboxyl-functionalized "diazole" heterocycles have been prepared and evaluated. Initially, a limited investigation of 4-arylimidazole-5-carboxylates led to 2-n-butyl-4-(2-holrophenyl)-1-[[2'-(1H-tetrazol-5-y1)biphenyl-4-y1]methyl]-1H-imidazole-5-carboxylic acid (I), which was found to be a highly potent antagonist of the rabbit aorta ATI receptor (IC50 0.55 nM). In conscious, normotensive rats, I at 0.1 mg/kg i.v. inhibited the pressor response to ATI by 88%, with a duration of >6 h. More extensively studied was an isosteric series of 3-alkyl-4-[2'-(1H-tetrazol-5-y1)biphenyl-4-

yl]methyl]-lH-pyrazole-5-carboxylates bearing aryl, alkyl, or aralkyl substituents at N1. These compds. were available in highly regioselective fashion via condensation of a substituted hydrazine hydrochloride with a 2-(methoxyimino)-4-oxoalkanoate intermediate. In vitro, the most potent pyrazolecarboxylic acids were II (R = Bu, Rl = 2,6-dichlorophenyl, 2-(trifluoromethyl)phenyl, benzyl, and phenethyl), all with IC50 values of 0.18-0.24 nM. Although less potent in the receptor assay, 3-n-propylpyrazolecarboxylic acids were at least as effective as their Bu counterpart in vivo. Several of the pyrazolecarboxylic acid derivs. demonstrated potent, long-lasting oral activity in rats. At 1 mg/kg po, the II (R = Bu, Rl = benzyl; R = Pr, Rl = 2,6-dichlorophenyl, 2,2,2-trifluoroethyl, and benzyl) analogs all gave 2/5% inhibition of the AII pressor response in the rat model, with duration of action >23 h.

IT 138733-03-6P 152713-36-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and angiotensin II antagonist activity of)

RN 138733-03-6 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 3-butyl-1-(2-pyridinyl)-4-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]- (CA INDEX NAME)

RN 152713-36-5 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 3-butyl-1-(2-pyridinyl)-4-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, ethyl ester (CA INDEX NAME)

IT 152713-67-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclization of, with azide, triazole derivative from) RN $\,$ 152713-67-2 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 3-buty1-4-[(2'-cyano[1,1'-bipheny1]-4yl)methyl]-1-(2-pyridinyl)-, ethyl ester (CA INDEX NAME)

L4 ANSWER 42 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1992:194308 CAPLUS

DOCUMENT NUMBER: 116:194308

ORIGINAL REFERENCE NO.: 116:32929a,32932a

TITLE: Preparation of 1-(2-pyridyl or

-pyrimidyl)5-hydroxypyrazoles as fungicidal materials

preservatives

INVENTOR(S): Sasse, Klaus; Schwamborn, Michael; Wachtler, Peter; Frie, Monika; Ludwig, Georg Wilhelm; Paulus, Wilfried;

Schmitt, Hans Georg PATENT ASSIGNEE(S): Bayer A.-G., Germany

SOURCE: Ger. Offen., 14 pp. CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
DE 4023488	A1	19920130	DE 1990-4023488	19900724		
EP 469357	A1	19920205	EP 1991-111537	19910711		
R: AT, CH, DE,	DK, FR	, GB, IT, LI	, SE			
US 5175176	A	19921229	US 1991-731680	19910717		
JP 04234385	A	19920824	JP 1991-203739	19910719		
US 5292744	A	19940308	US 1992-929652	19920812		
PRIORITY APPLN. INFO.:			DE 1990-4023488 A	19900724		
			US 1991-731680 A3	19910717		
OTHER SOURCE(S):	MARPAT	116:194308				

- AB Title compds. [I, R = H, (substituted) alkyl, aralkyl, alkoxy; Rl = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, aralkyl, alkoxy, alkylthio, aralkoxy, aralkylthio, aryloxy, arylthio, alkoxycarbonyl, aminocarbonyl; Rnl = alk(en)ylene; R2 = halo, NO2, cyano, (substituted) alkyl, alkoxy, alkylthio, alkoxycarbonyl, aminocarbonyl; n = 0-3; X = CH, NI, were prepared Thus, Et propionylacetate, 2-hydrazinopyridine, and EtOH were refluxed 3 h; KOCMe3 was added and the mixture was stirred 10 h to give title compound II. I showed min. inhibitory concns. of 5-50 mg/L against Alternaria tenuis.
- IT 140397-99-5P 140398-00-1P 140398-01-2P 140398-02-3P 140398-03-4P 140398-04-5P 140398-05-6P 140398-07-6P 140398-05-6P 140398-07-8P 140398-34-1P 140398-47-6P 140398-47-P 140398-49-8P 140398-50-1P
 - RL: SPN (Synthetic preparation); PREP (Preparation)
- (preparation of, as microbicidal materials preservative) RN 140397-99-5 CAPLUS
- N N

CN

Ph-CH2

- RN 140398-00-1 CAPLUS

1H-Pyrazol-5-ol, 4-(phenylmethyl)-1-(2-pyridinyl)- (CA INDEX NAME)

- RN 140398-01-2 CAPLUS
- CN 1H-Pyrazol-5-ol, 4-[(2-chloropheny1)methy1]-1-(2-pyridiny1)- (CA INDEX NAME)

- RN 140398-02-3 CAPLUS
- CN 1H-Pyrazol-5-ol, 4-[(2,4-dichlorophenyl)methyl]-1-(2-pyridinyl)- (CA INDEX NAME)

- RN 140398-03-4 CAPLUS
- CN 1H-Pyrazol-5-ol, 4-(4-chlorophenyl)-1-(2-pyridinyl)- (CA INDEX NAME)

140398-04-5 CAPLUS RN CN

1H-Pyrazol-5-ol, 4-[(4-methylphenyl)methyl]-1-(2-pyridinyl)- (CA INDEX NAME)

140398-05-6 CAPLUS RN

CN 1H-Pyrazol-5-ol, 4-[(4-methoxyphenyl)methyl]-1-(2-pyridinyl)- (CA INDEX NAME)

RN 140398-07-8 CAPLUS

CN 1H-Pyrazol-5-o1, 4-[(3-chloropheny1)methy1]-1-(2-pyridiny1)- (CA INDEX NAME)

RN 140398-08-9 CAPLUS

CN 1H-Pyrazol-5-ol, 4-[(4-bromophenyl)methyl]-1-(2-pyridinyl)- (CA INDEX NAME)

RN 140398-09-0 CAPLUS

CN 1H-Pyrazol-5-ol, 4-[(3-methylphenyl)methyl]-1-(2-pyridinyl)- (CA INDEX NAME)

RN 140398-10-3 CAPLUS

CN 1H-Pyrazol-5-ol, 4-[[4-(1,1-dimethylethyl)phenyl]methyl]-1-(2-pyridinyl)-(CA INDEX NAME)

10/551,709

RN 140398-34-1 CAPLUS

CN 1H-Pyrazol-5-ol, 3-phenyl-4-(phenylmethyl)-1-(2-pyridinyl)- (CA INDEX NAME)

RN 140398-47-6 CAPLUS

CN 1H-Pyrazol-5-ol, 3-methyl-4-phenyl-1-(2-pyridinyl)- (CA INDEX NAME)

RN 140398-48-7 CAPLUS

CN 1H-Pyrazol-5-ol, 3-methyl-4-(phenylmethyl)-1-(2-pyridinyl)- (CA INDEX NAME)

Ph-CH2 OH

RN 140398-49-8 CAPLUS

 $\texttt{CN} \qquad \texttt{1H-Pyrazol-5-ol, 3-methyl-4-(1-phenylethyl)-1-(2-pyridinyl)-} \qquad \texttt{(CA INDEX)} \\$

NAME)

140398-50-1 CAPLUS

ĊN 1H-Pyrazol-5-ol, 4-[1,1'-biphenyl]-4-yl-3-methyl-1-(2-pyridinyl)- (CA INDEX NAME)

INVENTOR(S):

L4 ANSWER 43 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:106284 CAPLUS 116:106284 DOCUMENT NUMBER: ORIGINAL REFERENCE NO.: 116:18003a,18006a

TITLE: Preparation of substituted pyrazoles, isoxazoles and

isothiazoles as angiotensin II antagonists Allen, Eric E.; Greenlee, William J.; MacCoss,

Malcolm; Ashton, Wallace T. PATENT ASSIGNEE(S): Merck and Co., Inc., USA SOURCE:

PCT Int. Appl., 171 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9115479	A1	19911017	WO 1991-US1952	19910327
W: CA, JP				
RW: AT, BE,	CH, DE, DK	, ES, FR,	GB, GR, IT, LU, NL, SE	
CA 2079343	A1	19911001	CA 1991-2079343	19910327
EP 523141	A1	19930120	EP 1991-907490	19910327
R: CH, DE,	FR, GB, IT	, LI, NL		

AB

JP 05505822 T 19930826 JP 1991-507326 19910327
PRIORITY APPLN. INFO: US 1990-501469 A 19900330
OTHER SQURCE(S): MARPAT 116:106284

(alkyl)sulfinyl, (alkyl)sulfonyl), CH(OH), O, CO, K = O, S, NH, (substituted) alkylamino, etc.; X = bond, CO, O, S, NH, etc.; R1 = HO2C, HO3S, C1-4 polyfluoroalkylsulfonylamino, H2NSO2, (HO)2P(O), (substituted) heterocyclyl, etc.; R2a, R2b = H, halo, H2N, O2N, C1-4 alkyl, C1-4 alkoxy, etc.; R3a = H, halo, C1-6 alkyl, C1-6 alkoxy, etc.; R3b = H, halo, O2N, C1-6 alkyl, hydroxy-C1-4-alkyl, etc.; R6 = C1-3 alkyl, C2-5 alkenyl, C2-5 alkynyl which can be substituted, R8 = H, HO, (alkyl)(dialkyl)amino, etc.; r = 1, 2] and their salts, as angiotensin II antagonists useful in treatment of hypertension, ocular hypertension, on certain CNS disorders (no data) are prepared 5-Amino-3-butyl-1-(2-chlorophenyl)-4-(2-tetrazol-5-ylbiphenyl-4yl)methyl]pyrazole (preparation given) in CC14 was diazotized to give the pyrazole derivative which was heated with NaCN in DMSO to give the nitrilepyrazole which was diluted with brine and extracted with ether to give the title pyrazole II. Pharmaceutical formulations comprising II are given.

Title compds. I [E = bond, (substituted) amino, (alkyl)thio,

IT 138733-03-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as angiotensin II inhibitor)

- RN 138733-03-6 CAPLUS
- CN 1H-Pyrazole-5-carboxylic acid, 3-butyl-1-(2-pyridinyl)-4-[[2'-(2H-tetrazol-5-v1)[1,1'-biphenyl]-4-v1]methyl]- (CA INDEX NAME)

L4 ANSWER 44 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN 1987:133797 CAPLUS

ACCESSION NUMBER: DOCUMENT NUMBER: ORIGINAL REFERENCE NO.:

106:133797 106:21747a,21750a

TITLE:

Preparation of 1-heteroaryl-4-arylpyrazole derivatives as bactericides and fungicides

INVENTOR(S):

Sasse, Klaus; Haenssler, Gerd; Schmitt, Hans Georg;

Paulus, Wilfried PATENT ASSIGNEE(S):

Bayer A.-G. , Fed. Rep. Ger. Ger. Offen., 22 pp. SOURCE: CODEN: GWXXBX

DOCUMENT TYPE:

Patent LANGUAGE: German FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3527157	A1	19870212	DE 1985-3527157	19850730
US 4772608	A	19880920	US 1986-886284	19860715
EP 212281	A1	19870304	EP 1986-109958	19860721
EP 212281	B1	19890906		
R: AT, BE, CH,	DE, FR		, NL	
AT 46160	T	19890915	AT 1986-109958	19860721
DK 8603606	A	19870131	DK 1986-3606	19860729
ZA 8605649	A	19870429	ZA 1986-5649	19860729
HU 43244	A2	19871028	HU 1986-3226	19860729
JP 62033171	A	19870213	JP 1986-177885	19860730
US 4806540	A	19890221	US 1987-99928	19870923
PRIORITY APPLN. INFO.:			DE 1985-3527157	A 19850730
			US 1986-886284	A3 19860715
			EP 1986-109958	A 19860721

OTHER SOURCE(S): GI

CASREACT 106:133797

AB Title compds. I and II (X = CH, N; R = H, alkyl; Rl = halo, OH, (un)substituted alkyl or alkowy, NO2, etc.; R2 = H, (un)substituted alkyl, cycloalkyl, aryl, or heterocyclyl, alkowy, alkylthio, etc.; Y = CO, SO2; n = 0, 1-5] are prepared as bactericides and fungicides.

1-Pyrid-2-yl-4-phenylpyrazolin-5-one was refluxed with Ac2O for 6 h to give I and II (R = Rl = H, R2 = Me, X = CH, Y = CO) (III and IV). III and IV were more effective in protecting rice against Pyricularia than was the standard Zineb.

II 107360-94-IP RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as microbicide)

RN 107360-94-1 CAPLUS

CN 1H-Pyrazol-5-ol, 4-phenyl-1-(2-pyridinyl)-, 5-acetate (CA INDEX NAME)

L4 ANSWER 45 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1971:87204 CAPLUS DOCUMENT NUMBER: 74:87204

DOCUMENT NUMBER: 74:87204

ORIGINAL REFERENCE NO.: 74:14157a,14160a

TITLE: Possibility of intramolecular hydrogen bonding in 1-[B-(2-pyridyl)ethyl]-5-amino(hydroxy) pyrazoles AUTHOR(S): Alieva, S. A.; Kolodyazhnyi, Yu. V.; Garnovskii, A. D.; Osipov, O. A.; Grandberg, I. I.; Krokhina, N. F. Rostov. -na-Donu Gos. Univ., Rostov-on-Don, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1970), (9),

1255-7

CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB The dipole moments of I (R = CH2Ph, R1 = Ph, R2 = 2-pyridyl, R3 = NH2), I (R = Ph, R1 = Me, R2 = 2-pyridyl, R3 = OH) and 14 other I were determined in dioxane and C6H6. The measured values agreed with those calculated on the basis of intramol. H bonds. Ir data is also discussed.

T 19551-22-5

RL: PRP (Properties)

(dipole moment of, intramol. hydrogen bonding in relation to)

RN 19551-22-5 CAPLUS

CN Pyridine, 2-[2-(5-amino-3-benzyl-4-phenylpyrazol-1-yl)ethyl]- (8CI) (CA INDEX NAME)

L4 ANSWER 46 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1970:466516 CAPLUS

DOCUMENT NUMBER: 73:66516

ORIGINAL REFERENCE NO.: 73:10894h,10895a

TITLE: Complexes of metals with nitrogen-containing ligands.

XIX. Complexes of tin tetrachloride with

1-pyridylpyrazoles and their 5-hydroxy(amino)

derivatives

AUTHOR(S): Garnovskii, A. D.; Kolodyazhnyi, Yu. V.; Alieva, S. A.; Krokhina, N. F.; Grandberg, I. I.; Osipov, O. A.;

Presnyakova, T. M.

CORPORATE SOURCE: Rostov.-na-Donu Gos. Univ., Rostov-on-Don, USSR SOURCE: Zhurnal Obshchei Khimii (1970), 40(5), 1114-20

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal Russian

LANGUAGE:

- From dipole moment and ir data it was concluded that 1-(2-pyridy1)pyrazole and its derivs, exist as angular isomers, in which (during complex) formation both N atoms may assume the otherwise unfavorable cis configuration. Dipole moments were tabulated from dielec. data in dioxane for 1-(pyridyl)pyrazoles with substituents selected from H, Me, PhCH2, p-H2NC6H4, p-MeC6H4, Et, Ph, and NH2; and 5-hydroxy or 5-amino derivs. of these with other substituents selected from H, Ph, Et, Bu, Me, p-MeOC6H4, and PhCH2. Several complexes of pyridylpyrazoles and
- (pyridylalkyl)pyrazoles with SnCl4 were prepared 19541-71-0DP, Pyridine, 2-(5-amino-3-benzyl-4-phenylpyrazol-1-yl)-, tin complexes 19551-22-5DP, Pyridine, 2-[2-(5-amino-3-benzyl-4-phenylpyrazol-1-yl)ethyl]-, tin complexes RL: SPN (Synthetic preparation); PREP (Preparation)
- (preparation of) 19541-71-0 CAPLUS RN
- CN Pyridine, 2-(5-amino-3-benzyl-4-phenylpyrazol-1-yl)- (8CI) (CA INDEX NAME)

RN 19551-22-5 CAPLUS

T. 4

CN Pyridine, 2-[2-(5-amino-3-benzyl-4-phenylpyrazol-1-yl)ethyl]- (8CI) (CA INDEX NAME)

ACCESSION NUMBER: 1970:110632 CAPLUS 72:110632

DOCUMENT NUMBER:

ORIGINAL REFERENCE NO.: 72:19963a,19966a

TITLE: Nitrogen-containing bisheterocyclic systems. I. Dipole moments and structure of 1-pyridylpyrazoles AUTHOR(S): Alieva, S. A.; Kolodyazhnyi, Yu. V.; Garnovskii, A.

D.; Osipov, O. A.; Grandberg, I. I.; Krokhina, N. F. CORPORATE SOURCE: Rostov.-na-Donu Gos. Univ., Rostov-on-Don, USSR SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1970), (1),

CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal LANGUAGE: Russian

For diagram(s), see printed CA Issue.

AB The dipole moments of 1-pyridyl-pyrazoles and their amino derivs. were determined in C6H6 at 25° with 5 + 10-3-2 + 10-4 mole fraction. Comparison of exptl. and vectorially calculated dipole moments shows that 1-pyridyl pyrazoles, and 1-(3- or 4-pyridyl)5-aminopyrazoles have non-planar configuration; the planar angle between the pyrazole and pyridine rings was calculated For 1-(2-pyridyl)-5-aminopyrazoles the planar trans configuration is assumed due to intramol. H bonding. The following data were obtained (R, R1, R2, position attachment of pyridine ring, and planar angle between two rings given): Me, H, Me, 2, 58°; Me, H, Me, 3, 84°; Me, H, Me, 4, 0°; Pr, Et, NH2, 3, 66°; PhCH2, Ph, NH2, 3, 56°; p-MeC6H4, H, NH2, 3, 80°; Et, Me,

NH2, 4, 0°; Me, H, Cl, 1, 0°; Me, H, NH2, 2, 0°; PhCH2, Ph, NH2, 2, 0°; Et, Me, NH2, 2, 0°; Pr, Et, NH2, 2,

0°; p-H2NC6H4, H, NH2, 2, 0°.[

19541-71-0

RL: PRP (Properties) (dipole moment of)

19541-71-0 CAPLUS RN

Pyridine, 2-(5-amino-3-benzyl-4-phenylpyrazol-1-yl)- (8CI) (CA INDEX CN NAME)

L4 ANSWER 48 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1969:11624 CAPLUS

DOCUMENT NUMBER: 70:11624 ORIGINAL REFERENCE NO.: 70:2178h,2179a

TITLE: Pyrazoles. LXV. Synthesis of a series of 5-hydroxy-

and 5-aminopyrazoles with nitrogen-containing

functional substituents

AUTHOR(S): Grandberg, I. I.; Krokhina, N. F.; Kondrat'ev, M. N. CORPORATE SOURCE: Mosk. S-Kh. Akad. im. Timiryazeva, Moscow, USSR SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1968), 2(7), 24-8

CODEN: KHFZAN; ISSN: 0023-1134

DOCUMENT TYPE: Journal LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB The synthesis of 5-aminopyrazoles is described. To a boiling mixture of

0.05 mole RNHNH2, 0.055 mole concentrated HC1 and 10 ml. H20 was added slowly under stirring 0.05 mole R1C(:NH)CHR2CN in 20 ml. iso-PrOH and the mixture was refluxed 20 min. on a H2O bath. After adding 60 ml. concentrated HCl, refluxing was continued 2 hrs. The solvent and excess HCl were evaporated in vacuo, the residue treated with an excess of 40% KOH and if the separated oil did not crystallize it was extracted with C6H6 or ether and distilled in vacuo. The following I were prepared (R, R1, R2, % vield, and b.p./mm. given): iso-Pr, Et, Me, 73.6, 116°/8; Et, Et, Me, 90.3, 130-5°/10; Me, Et, Me, 43, 130-5°/15; Me, Me, H, 12.6, 115-18°/8; (CH2)3NMe2, Me, H, 41, 155-63°/3. A mixture of 0.05 mole RNHNH2 and 0.05 mole β -keto ester was refluxed 12 hrs. on a water bath in 50 ml. tert-BuOH, 5 ml. H2O, and 5 ml. 50% AcOH, and the solvent was evaporated in vacuo. to give the following II (R, R1, R2, % yield, and m.p. given): α-C5H4N, CH2Ph, Ph, 59, 190°; (CH2)2C5H4N-γ, CH2Ph, Ph, 37.2, 148°; β-C5H4N, CH2Ph, Ph, 82.2, 198°; γ-C5H9NMe, Ph, H, 51.8, 105°; γ-C5H9NMe, CH2Ph, Ph, 50.4, 204°. Heating 0.04 mole α -, β - or γ-pyridylhydrazine in 10 ml. iso-PrOH 1 hr. on a water-bath with 0.04 mole acetylacetone gave the following III (R, % yield, and b.p./mm. given): γ-C5H4N, 63.5, 160°/20; α-C5H4N, 60.7, 130°/18; (CH2)2C5H4N-α, 77.9, 152-5°/15; β-C5H4N, 63.5, 152-4°/18; (CH2)2C5H4N-γ, 74.6, 173-5°/18. Pyrazole carbamates (IV) were prepared by refluxing 1 hr. an equimolar mixture of methyl isocyanatocarbamate and 5-aminopyrazole in absolute HCONMe2. The following IV were prepared (R, R1, R2, % yield, and m.p. given). (CH2) 2C5H4N-α, p-C6H4NHCON-HMe, H, 62, 227-8°; (CH2) 2C5H4N-γ, p-C6H4HCONHMe, H, 61, 227-8°; (CH2) 2C5H4N-α, CH2Ph, Ph, 58.8, 160-1°; (CH2) 2-C5H4N-α, C5H11, Bu, 54.8, 76-8°. 21018-65-5P 22301-80-0P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 21018-65-5 CAPLUS Pyrazol-5-ol, 3-benzyl-4-phenyl-1-(2-pyridyl)- (8CI) (CA INDEX NAME)

ΙT

RN

CN

RN 22301-80-0 CAPLUS

CN Urea, 1-[3-benzyl-4-phenyl-1-[2-(2-pyridyl)ethyl]pyrazol-5-yl]-3-methyl-(8CI) (CA INDEX NAME)

L4 ANSWER 49 OF 50 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1968:459155 CAPLUS

DOCUMENT NUMBER:

69:59155 ORIGINAL REFERENCE NO.: 69:11059a

TITLE: Pyrazoles. LXII. The synthesis of 5-aminopyrazole

series with potential physiological activity

AUTHOR(S): Grandberg, I. I.; Krokhina, N. F.

Mosk. Sel'skokhoz. Akad. im. Timiryazeva, Moscow, USSR

SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1968), 2(1), 16-22

CODEN: KHFZAN; ISSN: 0023-1134

DOCUMENT TYPE: Journal LANGUAGE: Russian

For diagram(s), see printed CA Issue.

EtCN (110 g.) in 150 cc. absolute Et20 was added carefully very slowly to 27.6 g. fine powdered Na in 150 cc. boiling Et2O, the mixture refluxed 8 hrs., and the product decomposed with 100 cc. H2O to give 27.5% RCH2C(:NH)CHRCN (I) (R = Me), b3 105-8°. Similarly, 30.8% I (R = H), 20.3% I (R = Et, and

19.3% I (R = Bu) were obtained. PhCH2CN (117 g.) was added dropwise to

11.5 g. Na in 130 cc. absolute iso-PrOH, the mixture heated 30 min. on a boiling

water bath, diluted with H2O, and extracted with Et2O, Et2O distilled, and unchanged PhCH2CN distilled with steam to give 29.7% PhCH2COCHPhCN, b3 230-40°, m. 91° (iso-PrOH) [Rf 0.73 on Al203 thin-layer in

20:1 CHCl3-MeOHl, and 15% PhCH2C(: NH)CHPhCN, b3 245-70°: Rf 0.67.

Iminonitrile (0.05 mole) in 20 cc. iso-PrOH was added slowly with stirring to a boiling mixture of 0.05 mole hydrazine, 0.055 mole concentrated HCl, and

cc. H2O, the mixture refluxed, 60 cc. concentrated HCl added, the mixture refluxed 2

hrs. and concentrated in vacuo, and the residue treated with 40% KOH to give I given in the 1st table. [TABLE OMITTED] Similarly, p-substituted 0-cyanoacetophenones gave I (R3 = H) given in the 2nd table. II (0.1 mole) was added slowly to 20 cc. N2H4.H2O, and 4 g. Raney Ni catalyst in 200 cc. boiling iso-PrOH, and the mixture refluxed 8 hrs. to give 86% I (R1 = R2 = p-H2NC6H4, R3 = H), m. 227-9° (alc.). [TABLE OMITTED]The preliminary results of the investigation of the physiol. activity of I

were pos. 19541-71-0P 19551-22-5P 19551-25-8P

20456-72-8P RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) RN 19541-71-0 CAPLUS

CN Pyridine, 2-(5-amino-3-benzyl-4-phenylpyrazol-1-yl)- (8CI) (CA INDEX NAME)

19551-22-5 CAPLUS

Pyridine, 2-[2-(5-amino-3-benzyl-4-phenylpyrazol-1-yl)ethyl]- (8CI) (CA INDEX NAME)

RN 19551-25-8 CAPLUS

CN Pyridine, 2-[2-(5-amino-3-benzyl-4-phenylpyrazol-1-yl)ethyl]-, tartrate (8CI) (CA INDEX NAME)

CM 1

CRN 19551-22-5 CMF C23 H22 N4

CM 2

CRN 87-69-4 CMF C4 H6 O6

Absolute stereochemistry.

RN 20456-72-8 CAPLUS

CN Pyridine, 2-(5-amino-3-benzyl-4-phenylpyrazol-1-yl)-, monohydrochloride (8CI) (CA INDEX NAME)

HC1

ACCESSION NUMBER:

DOCUMENT NUMBER:

```
ORIGINAL REFERENCE NO.: 60:8013e-h,8014a-c
TITLE:
                         Reactions of hydrazine derivatives. XXXIX. Addition of
                          hydrazine and substituted hydrazines to
                          2-vinvlpvridine
AUTHOR(S):
                          Kost, A. N.; Suminov, S. I.; Vinogradova, E. V.;
                         Kozler, V.
CORPORATE SOURCE:
                          State Univ., Moscow
SOURCE:
                          Zhurnal Obshchei Khimii (1963), 33(11), 3606-13
                          CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE:
                          Journal
LANGUAGE:
                          Unavailable
    cf. CA 55, 13423d; 59, 13964g. To 65 ml. 96% N2H4.H2O was added 25 ml.
     MeOH followed at 70-80° by 105 g. 2-vinylpyridine over 45-60 min.;
     after 8 hrs. at 80°, the mixture was left overnight and yielded
     65-6.5% 2-(hydrazinoethyl)pyridine (I), b12 139-42°, b4
     113-16°, n20D 1.5552, d20 1.055, which slowly decomposed even in the
     cold; dipicrate decomposed 145-6° (149-50° in preheated bath);
     di-HCl salt m. 146.5-8° p-nitrobenzylidene derivative m.
     118.5-19.5°; 2-hydroxynaphthaldehyde and salicylaldehyde gave
     colored hydrazones; treatment with Ph isothiocyanate gave
     N1-phenyl-N3-[2-(2-pyridyl)ethyl]thiosemicarbazide; excess PhNCS gave also
     some PhNHCSNHN(CH2CH2C5H4N)CSNHPh (probable structure), m.
     180.5-1.0°. I and Me2CO gave the isopropylidene derivative, b15
     146-7°, n20D 1.5315, d20 1.011 (dipicrate m. 151-2°). I and
     mesityl oxide in AcOH in 4 hrs. refluxing gave 52.5%
     3,5,5-trimethyl-1-[2-(2-pyridyl)ethyl]pyrazoline, bl2 153-7°, b4
     158-9.5°, n20D 1.5215, d20 1.005 (dipicrate m. 155-6°).
     Similarly I and AcCH2CO2Et in C6H6 gave after heating finally to
     70° 82% 3-methyl-1-[2-(2-pyridyl)ethyl]-5-pyrazolone, m.
     126-7°; similarly was prepared the 3-phenyl analog, m.
     125-5.5°. I and Et α-butylacetoacetate gave
     3-methyl-4-butyl-1-[2-(2-pyridyl)ethyl]pyrazolone, m. 75-6° (after
     freezing-out of Et20EtOH); picrate m. 121.5°. I and
     3-benzyl-2,4-pentanedione in 5 hrs. on a steam bath gave 89% yellow
     3,5-dimethyl-4-benzyl-1-[2-(2-pyridyl)ethyl]pyrazole, b3 189-93°,
     1.5690, 1.1961 (dipicrolonate m. 204-5°); similarly I and Ac2CH2
     gave 69% 3.5-dimethyl-1-[2-(2-pyridyl)ethyl]pyrazole (II), b2.5
     124-6°, 1.5398, 1.1458 (dipicrolonate m. 194-5°).
     3-Propyl-2, 4-pentanedione similarly gave
     3,5-dimethyl-4-propyl-1-[2-(2-pyridyl)ethyl]pyrazole, b3 148-52°,
     1.5269, 0.9766 (dipicrolonate m. 218-19^{\circ}). II in AcOH was heated on a steam bath with 30% H2O2 12 hrs. (with addition of fresh peroxide) and
     gave after evaporation 26% N-oxide, m. 248-9°. To a solution of Na in
     PRNHNH2 prepared at 96°, was added 2-vinylpyridine and after 6 hrs. gave after quenching in ice 83.8% 2-[2-(1-phenylhydrazino)ethyl]pyridine,
     b3.5 185-90°, 1.6105, (picrate m. 100-1°). This kept 1 day
     with 1-methyl-4-piperidone, then heated briefly, treated with alc. HCl,
     heated to boiling, and cooled overnight gave 95%
     9-[2-(2-pyridyl)ethyl]-3-methyl-1,2,3,4-tetrahydrocarboline, m.
     93-3.5°; HCl salt m. 190°; sulfate m. 150°. PhNHNH2
     and 2-vinylpyridine in 6:100 AcOH 20 hrs. at reflux gave after addition of
     KOH and extraction with CHC13-(CH2C1)2 29.3%
     2-[2-(2-phenylhydrazino)ethyl]pyridine, b3.5 159-63°, m.
     122-3° (crude), m. 124.5-5° (from MeOH), along with a glassy
     substance, b3 180-215°; when the reaction above was run in more
     concentrated aqueous AcOH, much tar formed. 2-Vinylpyridine added to AcNHNH2
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120° gave in 6 hrs. 63.5% 2-[2-(2-acetylhydrazino)ethyl]pyridine, b2 173-6° (picrate m. 101-2°). 2-Vinylpyridine added to BZNHNH2 in boiling BuOH and refluxed 1 day and kept 1-2 days gave after dilution with Bt20, a low yield N-benzoyl-N',N'-bis[2-(2-pyridyl)ethyl]hydrazine, m. 137-7.5° (dipicrate m. 174.5-5.0°); the yield was 37% when the refluxing in BuOH extended 20 hrs. and the mixture was concentrated Tetrahydroquinoline and 2-methyl-5-unylpyridine in the presence of hydroquinone were treated on a steam bath with Na and after 6 hrs. gave 42.6% 2-methyl-5-(N-tetrahydroquinolyl)ethylpyridine, b4 185-6° (picrate m. 199-200°). Similarly, indoline gave only a trace of an oily product, b3 191°; similar reaction in refluxing AcOH in 6 hrs. gave N-acetylindoline, m. 105-6°, only. Ultraviolet spectra of the products are reported. 94311-87-22. Pyridine, 2-[2-(4-benzyl-3,5-dimethylpyrazol-1-

II 94311-87-2P, Pyridine, 2-[2-(4-benzyl-3,5-dimethylpyrazol-1yl)ethyl]- 106278-65-7P, Pyridine,
2-[2-(4-benzyl-3,5-dimethylpyrazol-1-yl)ethyl]-, dipicrolonate

RL: PREP (Preparation)
(preparation of)

RN 94311-87-2 CAPLUS

CN Pyridine, 2-[2-[3,5-dimethyl-4-(phenylmethyl)-1H-pyrazol-1-yl]ethyl]- (CA INDEX NAME)

RN 106278-69-7 CAPLUS

CN Pyridine, 2-[2-[3,5-dimethyl-4-(phenylmethyl)-1H-pyrazol-1-yl]ethyl]-, compd. with 2,4-dihydro-5-methyl-4-nitro-2-(4-nitrophenyl)-3H-pyrazol-3-one (1:2) (CA INDEX NAME)

CM 1

CRN 94311-87-2 CMF C19 H21 N3

CM 2

CRN 550-74-3 CMF C10 H8 N4 O5

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